ExxonMobil Chemical Company

Alkyl Acetate C6 to C13 Category Analysis Report

For the

U.S. High Production Volume Chemical Challenge Program

Prepared by

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EXECUTIVE SUMMARY

ExxonMobil Chemical Company hereby submits the category summary report for the Alkyl Acetate C6 to C13 Category under the Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program (Program). The purpose of this report is to:

- Present results of an assessment to determine whether six complex mixtures can be adequately characterized with data presented in the Alkyl Acetate C6 to C13 Category test plan and new data developed as proposed in the test plan.
- Summarize the SIDS (Screening Information Data Set) physicochemical, environmental fate and effects, and human health HPV Program endpoints for the Alkyl Acetate C6 to C13 Category.
- Provide a description of manufacturing processes, potential exposure sources, and uses for C6 to C13 Alkyl Acetates.

ExxonMobil Chemical Company believes a category of Alkyl Acetates C6 to C13 is scientifically justifiable because their physicochemical and toxicological properties are similar or follow a predictable pattern based on chemical structure. Their structural similarity provides a predictable pattern for the following parameters: physicochemical properties, environmental fate and effects, and human health effects. The similarity is based on the following:

- A common structure [CH3C(=O)OR, which is an alkyl acetate ester where R represents various methyl-branched or methyl-branched and linear alkyl groups].
- An incremental and constant change across the category members, where for each member, R is composed predominantly of a single carbon (C) number (C6, C7, C8, C9, C10, or C13) as the main constituent.
- A common functional acetate ester group.
- The likelihood of similar breakdown products which result in structurally similar chemicals (e.g., acetic acid and C6 to C13 aliphatic alcohols).

The compiled test data prove adequate to support a screening-level hazard assessment for the category and its members, thereby allowing the assessment of untested members by interpolation between and extrapolation from tested members. Category members include:

- CAS #88230-35-7 Hexanol, acetate, branched and linear
- CAS #90438-79-2 Acetic acid, C6-8 branched alkyl esters
- CAS #108419-32-5 Acetic acid, C7-9 branched alkyl esters
- CAS #108419-33-6 Acetic acid, C8-10 branched alkyl esters
- CAS #108419-34-7 Acetic acid, C9-11 branched alkyl esters
- CAS #108419-35-8 Acetic acid, C11-14 branched alkyl esters

Exposure

Member substances of the Alkyl Acetate C6 to C13 Category are mainly used as solvents in such industries as lacquer, janitorial cleaning, and agricultural. Alkyl acetates are transported using tank cars, tank wagons, barges, and/or drums. Exposure to C6 to C13 alkyl acetates from manufacturing activities may occur at the workplace or during transport. Based on physical properties, potential workplace exposures would be through inhalation and dermal contact, which is controlled and minimized through the use of engineering controls, proper work procedures, and personal protective equipment.

At production sites, potential exposure to Alkyl Acetates C6 to C13 in the environment is low because there are no direct releases to the environment and process, storage, and handling facilities are enclosed.

Human Health

Members of the Alkyl Acetate C6 to C13 Category have a low order of toxicity by the oral and dermal routes of exposure. Oral LD_{50}s range from >2000 to 10,000 mg/kg and dermal LD_{50}s range from >2000 to 3160 mg/kg. Thus, the acute oral and dermal toxicity for the Alkyl Acetate C6 to C13 Category is well characterized.

Studies have demonstrated that the members of the Alkyl Acetate C6 to C13 Category are mildly to moderately irritating to the skin and only mildly irritating to the eyes. Thus, the skin and eye irritation potential for the Alkyl Acetate C6 to C13 Category has been well characterized and no further studies are proposed.

Members of the Alkyl Acetate C6 to C13 Category are not expected to be skin sensitizers in animals or humans as a structurally similar chemical, 1-hexanol, did not induce sensitising reactions in guinea pigs or humans. Data are not available to assess the potential for respiratory tract sensitisation in animals or humans. However, since the members of this category are not expected to be skin sensitizers, they are also not expected to be respiratory tract sensitizers. Additionally, due to the low to moderate vapour pressure of members of this category, potential atmospheric exposure is expected to be limited.

A repeated dose oral toxicity study was conducted with C6 branched and linear alkyl acetate ester in rats. In this study, the rats received 0, 100, 500, and 1000 mg/kg of test material per day for 28 days by oral gavage. The repeated oral administration of C6 branched and linear alkyl acetate ester to rats for 28 days did not produce any adverse effects at any dose level tested. The No Observed Adverse Effect Level (NOAEL) in this study was 1000 mg/kg/day. Repeated dose oral toxicity studies were also conducted with C7-C9 and C11-C14 branched alkyl acetate esters. In these studies, rats received 0, 100, 500, and 1000 mg/kg of test material by oral gavage, 5 days/week for 13 weeks. No significant treatment-related effects were observed during these studies. Although terminal liver and kidney weights were elevated in a dose-related manner, they were considered to be adaptive changes and not indicative of toxic effects. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy only in high dose male rats in both studies. This is consistent with alpha-2-μ-globulin effects. This effect is known to be male rat specific and is not relevant for humans. Histopathology of all other tissues from high dose animals showed normal morphology. Based on these results, the No Observed Adverse Effect Level for C7-C9 and C11-C14 branched alkyl acetate esters is 1000 mg/kg/day. In summary, based on the results of the repeated-dose studies conducted in animals, the members of the Alkyl Acetate C6 to C13 Category appear to have a low order of subchronic toxicity.

Members of the Alkyl Acetate C6 to C13 Category appear to have a low potential for mutagenic effects. C6 branched and linear alkyl acetate, C6-C8 branched alkyl acetate ester, C7-C9 branched alkyl acetate, and C11-C14 branched alkyl acetate ester were all tested in an Ames Assay in 5 strains of *Salmonella typhimurium* either in the presence or absence of metabolic activation. None of the materials tested were mutagenic in any of the *Salmonella* strains tested. In addition, C6 branched and linear alkyl acetate and C6-C8 branched alkyl acetate ester were tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. Both materials were considered to be negative for inducing chromosome aberrations under the conditions of the assay. *In vivo* mammalian bone marrow micronucleus assays were also conducted in CD-1 mice with C7-C9 branched alkyl ester and C11-C14 branched alkyl acetate ester. Neither material induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Thus, both materials were considered to be non-mutagenic under the conditions of this assay. Based on the above data, the mutagenic potential for the Alkyl Acetate C6 to C13 Category has been well characterized. By read-across, these data also support characterizing the untested members of this category as having a low potential for carcinogenicity.

Developmental toxicity studies were conducted in female Sprague-Dawley rats by the oral route of exposure with C7-C9 and C11-C14 branched alkyl acetate esters. Exposure of rats to the C7-C9 branched alkyl acetate ester resulted in slight increases in fetal malformations and embryotoxicity at the highest dose tested, i.e., 1000 mg/kg. However, as this dose produced maternal toxicity, the C7-C9 branched alkyl acetate ester should not be considered as a selective developmental toxicant. Exposure of rats to the C11-C14 branched alkyl esters produced maternal toxicity at the two highest doses tested, 1300 and 2500 mg/kg. However, there were no statistically significant deleterious effects on fetal survival, body weight, or crown-rump length and no evidence of treatment-related malformations. Thus, the C11-C14 branched alkyl acetate ester is not a selective developmental toxicant. Based on these results, the members of the Alkyl Acetate C6 to C13 Category appear to have a low order of developmental toxicity.

In conclusion, members of the Alkyl Acetate C6 to C13 Category have a low order of acute toxicity, are mild to moderate skin irritants, are mild reversible eye irritants and are not expected to produce skin or respiratory tract sensitization. Subchronic studies have also shown a low order of toxicity. The only effect observed upon microscopic evaluation in these studies was evidence of mild tubular nephropathy in the high-dose males. This effect is known to be male rat specific and is not relevant for humans. Testing in a variety of *in vitro* and *in vivo* genotoxicity assays has not shown any mutagenic activity with or without metabolic activation. Based on these negative genotoxicity data, category members are expected to have a low potential for carcinogenicity. Reproductive/ developmental testing has shown fetal effects in some studies, but only at doses that produced overt maternal toxicity. Thus, these data support that members of this category are not selective reproductive toxicants. Taken in concert, these data show that the toxicity of members in the Alkyl Acetate C6 to C13 Category, for the endpoints discussed, has been well characterized and support an overall low hazard assessment for category members.

Environment

In spite of their low to moderate vapour pressure, results of distribution modelling show that category members will partition predominantly to the air compartment, with the exception of acetic acid, C11-14 branched alkyl esters, which is expected to partition predominantly to the soil compartment. The air compartment is a primary compartment for these substances because the partitioning results are based on the chemical being at equilibrium, which does not show the period of time to reach this state. These results do suggest that assessment of these substances should not overlook their fate in the air where they have the potential to partition. Volatilization to the air from aqueous and terrestrial habitats is expected to occur at appreciable rates for most of these substances, and once in the air, they have the potential to rapidly degrade through indirect photolytic processes mediated primarily by hydroxyl radicals. This can be a significant route of loss and therefore a significant degradation process for members of this category. Aqueous photolysis and hydrolysis will not contribute to the transformation of category constituents in aquatic environments because they are either poorly or not susceptible to these reactions.

Biodegradability of the alkyl acetates has been evaluated with standard 28-day test guidelines. The results from these studies show that the alkyl acetates are subject to microbial degradation under aerobic conditions and that all but the C11-C14 branched alkyl acetate ester are expected to biodegrade at rapid rates, greater than 77% in 28 days.

Member substances of the Alkyl Acetate C6 to C13 Category have been shown to exhibit low to moderate acute aquatic toxicity. This assessment is supported by the results of aquatic toxicity studies for several organisms. Members ranging from the C6 branched and linear alkyl acetate ester to the C9-C11 branched alkyl acetate ester are expected to produce a relatively narrow range of moderate acute toxicity to freshwater aquatic organisms in the range of 7 to 40 mg/L. In comparison, the C11-C14 branched alkyl acetate is not expected to produce acute aquatic toxicity to freshwater fish and invertebrates, or toxicity to freshwater algae, based on results of studies for this

substance. The lack of toxicity is due to its comparatively lower water solubility, which limits the exposure of aquatic organisms to soluble fractions of this substance.

Category members have a low potential to bioaccumulate in aquatic species based on a calculated bioconcentration factor range of 30 to 754 (log BCF = 1.5 to 2.9).

Category members are expected to be removed in wastewater treatment facilities. A predominant mechanism accounting for their removal is biodegradation, followed with partitioning or sorbtion to sludge solids contributing to the remaining loss.

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1 IDENTITY

1.1 Identification of the Category

For purposes of the U.S. High Production Volume (HPV) Chemical Challenge Program (Program), the Alkyl Acetate C6 to C13 Category test plan submitted in December 2000 (ExxonMobil, 2000) included 6 Chemical Abstracts Service (CAS) registration numbers (RNs) (Table 1). The test plan identified existing data and additional data needed, based on an extensive technical review of the category, to adequately characterize the 6 chemicals for the HPV Program endpoints. This category analysis report summarizes HPV Program data for the Alkyl Acetate C6 to C13 Category, which contains 6 CAS RNs.

Table 1. CAS RN, CAS RN Name, Structure, Molecular Weight, and Synonyms of Members in the Alkyl Acetate C6 to C13 Category

CAS RNs with TSCA Names:	88230-35-7	Hexanol, acetate, branched and linear
	90438-79-2	Acetic acid, C6-8 branched alkyl esters
	108419-32-5	Acetic acid, C7-9 branched alkyl esters*
	108419-33-6	Acetic acid, C8-10 branched alkyl esters*
	108419-34-7	Acetic acid, C9-11 branched alkyl esters*
	108419-35-8	Acetic acid, C11-14 branched alkyl esters
CAS RNs with Molecular Formulas:	88230-35-7	C8H16O2
	90438-79-2	C9H18O2
	108419-32-5	C10H20O2
	108419-33-6	C11H22O2
	108419-34-7	C12H24O2
	108419-35-8	C15H30O2
CAS RNs with Structural Formulas:	88230-35-7	CH3-COO-(CH2)5-CH3
	90438-79-2	CH3-COO-(CH2)6-CH3
	108419-32-5	CH3-COO-(CH2)7-CH3
	108419-33-6	CH3-COO-(CH2)8-CH3
	108419-34-7	CH3-COO-(CH2)9-CH3
	108419-35-8	CH3-COO-(CH2)12-CH3
	(general structures; contain various methyl branching patterns)	

* Not HPV substances, but included to facilitate a category evaluation

Table 1. Continued

CAS RNs with Molecular Weights:	88230-35-7	144.2
	90438-79-2	158.2
	108419-32-5	172.0
	108419-33-6	186.3
	108419-34-7	200.3
	108419-35-8	242.0
CAS RNs with Synonyms:	88230-35-7	C6 branched and linear alkyl acetate ester; oxo-hexyl acetate
	90438-79-2	C6-C8 branched alkyl acetate ester; oxo-heptyl acetate
	108419-32-5	C7-C9 branched alkyl acetate ester; oxo-octyl acetate
	108419-33-6	C8-C10 branched alkyl acetate ester; oxo-nonyl acetate
	108419-34-7	C9-C11 branched alkyl acetate ester; oxo-decyl acetate
	108419-35-8	C11-C14 branched alkyl acetate ester; oxo-tridecyl acetate

1.2 Purity/Impurities/Additives

Hexanol acetate, branched and linear (CAS RN 88230-35-7)

Commercial hexanol acetate, branched and linear, is a clear, colourless liquid with a sweet ester odor and a typical purity of 97%. The commercial substance typically consists of branched and linear C6 isomers of hexyl acetate esters; the composition and CAS registry number depend on the alcohol feedstock. Hexanol acetate, methyl-branched and linear does not contain additives.

Acetic acid, C6-8 branched alkyl esters (CAS RN 90438-79-2)

Commercial acetic acid, C6-8 branched alkyl esters, is a clear, colourless liquid with a sweet ester odor and a typical purity of >99%. The commercial substance typically consists of methyl-branched isomers of C6 to C8 acetate esters (predominantly C7); the composition and CAS registry number depend on the alcohol feedstock. Acetic acid, C6-8 methyl-branched alkyl ester does not contain additives.

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

Commercial acetic acid, C7-9 branched alkyl esters, is a clear, colourless liquid with a sweet ester odor and a typical purity of >98%. The commercial substance typically consists of methyl-branched isomers of C7 to C9 acetate esters (predominantly C8); the composition and CAS registry number depend on the alcohol feedstock. Acetic acid, C7-9 methyl-branched alkyl ester does not contain additives.

Acetic acid, C8-10 branched alkyl esters (CAS RN 108419-33-6)

Commercial acetic acid, C8-10 branched alkyl esters, is a clear, colourless liquid with a sweet ester odor and a typical purity of >99%. The commercial substance typically consists of methyl-branched isomers of C8 to C10 acetate esters (predominantly C9); the composition and CAS registry number depend on the alcohol feedstock. Acetic acid, C8-10 methyl-branched alkyl ester does not contain additives.

Acetic acid, C9-11 branched alkyl esters (CAS RN 108419-34-7)

Commercial acetic acid, C9-11 branched alkyl esters, is a clear, colourless liquid with a sweet ester odor and a typical purity of >99%. The commercial substance typically consists of methyl-branched isomers of C9 to C11 acetate esters (predominantly C10); the composition and CAS registry number depend on the alcohol feedstock. Acetic acid, C9-11 methyl-branched alkyl ester does not contain additives.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

Commercial acetic acid, C11-14 branched alkyl esters, is a clear, colourless liquid with a sweet ester odor and a typical purity of >99%. The commercial substance typically consists of methyl-branched isomers of C11 to C14 acetate esters (predominantly C13); the composition and CAS registry number depend on the alcohol feedstock. Acetic acid, C11-14 methyl-branched alkyl ester does not contain additives.

Table 2 lists approximate carbon number distributions for members of the Alkyl Acetates C6 to C13 Category.

Table 2. Approximate Carbon Number Distribution of Members in the Alkyl Acetate C6 to C13 Category

Category Member	CAS Number	Composition (wt. %)
Hexanol, acetate, branched and linear (C6-rich)	88230-35-7	C6 >95% Low levels of C7, C8
Acetic acid, C6-8-branched alkyl esters (C7-rich)	90438-79-2	C7 >85% C6, C8 >2 to 15%
Acetic acid, C7-9-branched alkyl esters (C8-rich)	108419-32-5	C8 >90% C7, C9 >2 to 10% Low levels of C6, C10
Acetic acid, C8-10-branched alkyl esters (C9-rich)	108419-33-6	C9 >75% C10 >15% C8 >2% Low levels of C6, C7
Acetic acid, C9-11-branched alkyl esters (C10-rich)	108419-34-7	C10 >85% C9, C11 >2 to 15% Low levels of C6, C7, C8
Acetic acid, C11-14-branched alkyl esters (C13-rich)	108419-35-8	C12, C13 combined 40 to 96% C11 >2% Low levels of C9, C10, C14

1.3 Physico-Chemical properties

Physico-chemical data (i.e.; melting point, boiling point, vapor pressure, water solubility, and K_{ow}) for selected components in the Alkyl Acetate C6 to C13 Category were calculated using the EPIWIN© model (EPIWIN, 1999), as discussed in the EPA document titled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program." These data are presented as ranges, based on the chemical components selected to represent each alkyl acetate substance. In addition, measured data for some of these endpoints are also provided for selected alkyl acetate substances where available.

Table 3. Selected Physical Properties of Members in the Alkyl Acetate C6 to C13 Category

CAS Number	Category Member	Boiling Range (°C)[1]	Melting Point (°C)[2]	Vapor Pressure (mm Hg @ 25°C)[2]	Density (@ 20°C)[1]	Log K_{ow}[2]	Water Solubility (mg/L @ 25°C)[2]
88230-35-7	Hexanol, acetate, branched and linear	164-176	-59	1.45	0.87	2.83	309
90438-79-2	Acetic acid, C6-8 branched alkyl esters	176-200	-50	0.51	0.87	3.32	102
108419-32-5	Acetic acid, C7-9 branched alkyl esters	186-215	-30	0.70	0.87	3.66	45
108419-33-6	Acetic acid, C8-10 branched alkyl esters	205-235	-20	0.26	0.87	4.15	14.5
108419-34-7	Acetic acid, C9-11 branched alkyl esters	220-250	-8.8	0.10	0.87	4.65	4.7
108419-35-8	Acetic acid, C11-14 branched alkyl esters	240-285	-2	0.01	0.87	6.05	0.2

[1] Measured values

[2] Values calculated using EPIWIN model

1.4 Category Justification

The Alkyl Acetate C6 to C13 Category is a group of substances whose physicochemical and toxicological properties are very similar and follow a regular pattern as a result of structural similarity. The production of the alkyl acetate family involves the reaction of aliphatic, monohydric alcohols with acetic acid to form the corresponding acetate esters.

$$ROH + CH3COOH \rightarrow CH3COOR + H2O$$

Their structural similarity provides a predictable pattern for the following parameters: physicochemical properties, environmental fate and effects, and human health effects. The similarity is based on the following:

- A common structure [CH3C(=O)OR, which is an alkyl acetate ester where R represents various methyl-branched or methyl-branched and linear alkyl groups].
- An incremental and constant change across the category members, where for each member, R is composed predominantly of a single carbon (C) number (C6, C7, C8, C9, C10, or C13) as the main constituent.
- A common functional acetate ester group.
- The likelihood of similar breakdown products which result in structurally similar chemicals (e.g., acetic acid and C6 to C13 aliphatic alcohols).

Although the category is characterized as C6 to C13, one of the substances, acetic acid C11-14 branched alkyl ester (CAS #108419-35-8), contains very low levels of C14 (Table 2), which does not influence the overall assessment of this category.

2 GENERAL INFORMATION ON EXPOSURE

Member substances of the Alkyl Acetate C6 to C13 Category are mainly used as solvents in such industries as lacquer, janitorial cleaning, and agricultural. Alkyl acetates are transported using tank cars, tank wagons, barges, and/or drums. Exposure to C6 to C13 alkyl acetates from manufacturing activities may occur at the workplace or during transport. Based on physical properties, potential workplace exposures would be through inhalation and dermal contact, which is controlled and minimized through the use of personal protective equipment.

At production sites, potential exposure to Alkyl Acetates C6 to C13 in the environment is low because there are no direct releases to the environment and process, storage, and handling facilities are enclosed.

2.1 Production and Use Pattern

Category members are made in the esterification process by reacting hexanol with acetic acid in the presence of a catalyst, followed by azeotropic distillation (Aguilo, et al, 1984). A major use of the alkyl acetates is as solvents in lacquers and agricultural products (Clayton, 1994). Select members have also been used in janitorial cleaning and paint products.

2.2 Environmental Exposure and Fate

There is no information on environmental concentrations for substances in the Alkyl Acetate C6 to C13 Category. Measurable concentrations would not be anticipated in the general environment because of their rapid rate of biodegradation.

2.2.1 Sources of Environmental Exposure

Alkyl Acetate C6 to C13 Category substances are mainly used as solvents. They can enter the environment through application of agricultural and paint products in which they can be a component, and through the disposal of solid waste. Once in the environment they are expected to biodegrade rapidly. Henry's Law constant, a measure of the potential of a molecule to evaporate from open water, indicates that the molecules comprising category substances will generally volatilise at appreciable rates. However, once in air, these molecules would be subject to rapid atmospheric degradation via hydroxyl radical attack with calculated half-lives of less than 24 hours.

2.2.2 Photodegradation

Results from the Mackay Level I distribution model (Mackay, 1998) show that category members will partition predominantly to the air compartment (73 to 93%) at equilibrium with the exception of acetic acid, C11-14 branched alkyl esters, which is expected to partition predominantly to the soil compartment (approximately 74%). Therefore, indirect photodegradation as mediated by hydroxyl radical ($OH^{\cdot}$) attack in the air can significantly contribute to the potential overall degradation of alkyl acetate esters in the environment. Because of their lower potential to partition to the water compartment, direct photolysis, which occurs primarily in solution, may not significantly contribute to the photolytic degradation of category members in the aqueous environment.

Indirect Photolysis

In air, a chemical can react with photosensitised oxygen in the form of $OH^{\cdot}$ or ozone (O_3). These reactions can result in a degradative change in the parent chemical that can ultimately lead to its

complete degradation. Substances in the Alkyl Acetate C6 to C13 Category have the potential to rapidly react with OH^- in air, which can be a predominant daylight atmospheric degradation process for this chemical.

Potential OH^- reaction rate and atmospheric chemical half-life is calculated based on an average OH^- radical concentration. The atmospheric oxidation potential model (EPIWIN, 1999; Meylan and Howard, 1993) calculates a rate constant for the Alkyl Acetate C6 to C13 Category members ranging from 7.4E-12 to 18.7E-12 $cm^3mol^{-1}s^{-1}$ and an average atmospheric half-life ranging from 17.3 to 6.9 hours or 1.4 to 0.57 days, respectively. These values are based on a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated). The rate constants were calculated using an average global OH^- concentration of 1.5E6 OH^-/cm^3.

These data indicate that indirect photodegradation of Alkyl Acetate C6 to C13 Category substances can occur at a moderate to rapid rate, and, based on their vapour pressure, has the potential to contribute significantly to their overall degradation in the environment.

Direct Photolysis

Direct photochemical degradation in aqueous solution occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. A prerequisite for direct photodegradation is the ability of one or more bonds within a chemical to absorb ultraviolet (UV)/visible light in the 290 to 750 nm range. Light wavelengths longer than 750 nm do not contain sufficient energy to break chemical bonds, and wavelengths below 290 nm are shielded from the earth by the stratospheric ozone layer.

An approach to assess the potential for a substance to undergo photochemical degradation is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by constituent molecules (Zepp and Cline, 1977). Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis and will not contribute to the degradation of alkyl acetate esters in the aquatic environment.

2.2.3 Stability in Water

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond, thereby changing the parent chemical. Chemicals that are susceptible to hydrolysis contain functional groups that can be displaced by a nucleophilic substitution reaction. Potentially hydrolyzable groups include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Harris, 1982).

Studies to evaluate hydrolytic potential as a function of pH were performed using two members of the Alkyl Acetate C6 to C13 Category; hexanol, acetate, branched and linear (EMBSI, 1995a) and acetic acid, C6-8 branched alkyl esters (EMBSI, 1997a). Both studies were conducted following OECD 111 test guidelines at 3 relevant pH values (4, 7, and 9) and varying temperatures. The results of these studies indicate that hydrolysis is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 25°C and the pH is at or below 7. Therefore, hydrolysis will not contribute to their removal from the environment.

2.2.4 Transport between Environmental Compartments

Fugacity-based multimedia modelling provides basic information on the relative distribution of a chemical between selected environmental compartments (i.e., air, soil, water, sediment, suspended sediment, and biota). Fugacity is a physical chemistry concept and can be regarded as the "escaping tendency" of a chemical from a phase (environmental compartment). A widely used fugacity model is the EQC (Equilibrium Criterion) Level I model (Mackay *et al.,* 1996; Mackay, 1998). This model requires the input of basic physicochemical parameters such as molecular weight, melting point, vapor pressure, water solubility, log K_{ow}.

The Mackay Level I fugacity model is a steady state, equilibrium model that calculates a chemical's distribution into the 6 compartments listed above, based on the physicochemical data listed in Table 3. The parameters of the 6 compartments are defined in the model and the percent distribution results are based on a chemical achieving partitioning equilibrium between the compartments. Chemical degradation and advection are not considered within the model.

Results of the Mackay Level I environmental distribution model suggest that alkyl acetates will partition primarily to the air (Table 4) with the exception of acetic acid, C11-14 branched alkyl esters (Table 5) which is expected to partition predominantly to the soil compartment. These results can be explained in part by the vapour pressure (1.93 to 0.13 hPa) and log K_{ow} (2.8 to 4.7) values of category members in the C6 to C10 range, and the lower vapour pressure (0.013 hPa) and higher log K_{ow} (6.1) values for the C11-14 branched alkyl ester.

Table 4. Environmental Distribution as Calculated by the Mackay (1998) Level I Fugacity Model for Select Members in the Alkyl Acetate C6 to C13 Category

Environmental Compartment	Percent Distribution*
Air	73.4 to 93.3
Soil	3.0 to 25.3
Water	0.6 to 5.0
Sediment	<0.1 to 0.6
Suspended Sediment	< 0.02
Biota	< 0.01

*Distribution reflects the range of the C6 to C11 category members.

Table 5. Environmental Distribution as Calculated by the Mackay (1998) Level I Fugacity Model for the Highest Molecular Weight Member of the Alkyl Acetate C6 to C13 Category

Environmental Compartment	Percent Distribution
Soil	74.0
Air	24.2
Sediment	1.6
Suspended Sediment	0.05
Water	< 0.07
Biota	< 0.01

Henry's Law constants (HLCs) representing potential volatility from water were calculated for constituent chemicals within this category. The HLCs for category members range from 90.2 to 1573 Pa-m^3/mole (Table 6). These data suggest that category members would volatilize from water and terrestrial environments at appreciable rates. Henry's Law constants are based on vapor pressure and water solubility values cited in Table 3, and molecular weights cited in Table 1.

Table 6. Calculated Henry's Law Constants of Members in the Alkyl Acetate C6 to C13 Category

CAS Number	Category Member	Henry's Law Constant (Pa-m^3/mole)*
88230-35-7	Hexanol, acetate, branched and linear (C6-rich)	90.2
90438-79-2	Acetic acid, C6-8 branched alkyl esters (C7-rich)	105.5
108419-32-5	Acetic acid, C7-9 branched alkyl esters (C8-rich)	356.6
108419-33-6	Acetic acid, C8-10 branched alkyl esters (C9-rich)	445.8
108419-34-7	Acetic acid, C9-11 branched alkyl esters (C10-rich)	566.8
108419-35-8	Acetic acid, C11-14 branched alkyl esters (C13-rich)	1573.0

* Based on the predominant component.

2.2.5 Biodegradation

Biodegradation data are available for four category members, which show that these substances are rapidly biodegraded, with the exception of the highest molecular weight substance. The C11-C14 branched alkyl acetate ester has been shown to biodegrade at a moderate rate, which suggests that although it is not expected to degrade at a rate equivalent to the lighter molecular weight alkyl acetate ester substances, it also will not persist in the environment.

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

Following procedures outlined by USEPA test guidelines (EPA OTS 796.3100), using a non-acclimated activated sludge, sewage, and soil medium, C6 branched and linear alkyl acetate ester was shown to biodegrade rapidly in 28 days. The procedures followed the Gledhill Shake Flask Method. Based on theoretical carbon dioxide values and the cumulative carbon dioxide produced

by the test chemical, the study reported 76.9% biodegradation in the 28-day period (EMBSI, 1994a).

Acetic acid, C6-8 branched alkyl esters (CAS RN 90438-79-2)

In a manometric respirometry (OECD 301F) study, using non-acclimated inocula, C6-8 branched alkyl acetate esters was shown to biodegrade 77% in 28 days (EMBSI, 1998a). The results of the study are based on O_2 consumption.

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

No data are available.

Acetic acid, C8-10 branched alkyl esters (CAS RN 108419-33-6)

No data are available.

Acetic acid, C9-11 branched alkyl esters (CAS RN 108419-34-7)

In another manometric respirometry study, using a non-acclimated inocula, C9-11 branched alkyl acetate esters was shown to biodegrade 84.7% in a 28-day period (EMBSI, 1996a). The results of this study are based on O_2 consumption.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

Biodegradability of C11-14 branched alkyl acetate esters was examined following procedures outlined in USEPA test guidelines (EPA 560/6-83-003). In this study, the inoculum was acclimated to the esters for 14 days prior to study initiation. The media consisted of mineral salts solutions, pond sediment, activated sludge, distilled water, and small amounts of the test chemical. By Day 28, 31% biodegradation of the test chemical was observed (BioDynamics, 1985a). These results are based on CO_2 evolution.

2.2.6 Bioaccumulation

Using the BCFWIN estimation program (EPIWIN, 1999), bioconcentration factor (BCF) values range from 30 to 754 (log BCF = 1.5 to 2.9). These data suggest that category members have a low potential to bioaccumulate in aquatic species.

2.2.7 Other Information on Environmental Fate

Using the EPIWIN v.3.04 estimation program, members of the Alkyl Acetate C6 to C13 Category are expected to be removed from wastewater treatment facilities >95%. The predominant mechanism accounting for removal in a wastewater treatment facility is biodegradation, with partitioning of the esters to sludge accounting for the remaining loss.

2.3 Human Exposure

2.3.1 Occupational Exposure

Limited workplace exposure data are available for members of the Alkyl Acetate C6 to C13 Category. Workplace exposure to these alkyl acetates can occur through inhalation (primary route) and dermal contact (EMBSI, 1998b), which is controlled and minimized through the use of engineering controls, proper work procedures, and personal protective equipment. Potential for worker exposure exists during blending operations, maintenance, turnarounds, sample collection, and tank and barge loading. Limited air sampling data suggest that concentrations are well below 50

ppm (EMBSI, 1998b) for an 8-hour TWA (time-weighted average). This level equates to approximately 10 mg/m^3 for C6 to C13 alkyl acetate aerosol (ExxonMobil, 2003a).

2.3.2 Consumer Exposure

Consumer exposure is expected to be low. Exposure can occur through the use of finished products (*i.e.* paints, coatings, and agricultural products) that contain category members. Paints can contain approximately 6% alkyl acetate, as solvent (EMBSI, 1998c). In the paint drying process, nearly all of the alkyl acetate solvent is expected to evaporate to the atmosphere. The concentration of alkyl acetate in the air is expected to be insignificant due to dispersion and rapid atmospheric degradation rates.

3 HUMAN HEALTH HAZARDS

3.1 Effects on Human Health

3.1.1 Toxicokinetics, Metabolism and Distribution

The initial metabolic hydrolysis of the alkyl acetates results in reversal of the synthesis reaction. Metabolism of the alkyl acetates is catalyzed by esterases to yield acetic acid and the corresponding aliphatic alcohol. Alcohol residues liberated by esterases, would likely be broken down by mitochondrial beta-oxidation or by cytochrome P450 mediated omega and omega-minus-one oxidation (may be followed by beta-oxidation). The alcohol undergoes various oxidative steps to yield other alcohols, ketones, aldehydes, carboxylic acids and carbon dioxide (Mann, 1987). Because alcohols are the primary metabolites of alkyl acetates, data on alcohols are very useful to address the toxicologic properties of alkyl acetates. Data for monohydric, aliphatic alcohols show a systematic variation according to molecular weight in a manner similar to many other homologous series (Monick, 1968). The body handles aliphatic hydrocarbons in a similar manner via oxidative conversion to alcohols, ketones, and eventual elimination as carbon dioxide and carboxylic acids (Wislocki et al, 1980). The undegraded alcohols can be conjugated either directly or as a metabolite with glucuronic acid, sulfuric acid, or glycine and are rapidly excreted (Lington and Bevan, 1994). Acetyl residues liberated by the esterases would enter intermediary metabolism pathways, be broken down and excreted as carbon dioxide and water. Intermediate aldehydes could be reactive and bind with DNA and/or proteins. Glucuronidation and glutathione conjugation are possible means of rapid elimination (Mann, 1987).

3.1.2 Acute Toxicity

Studies in Animals

Oral

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

In this pre-GLP study, 5 male Sprague-Dawley rats received 34.6, 120, 417, 1450, 5000, or 10,000 mg/kg of the test material as a single dose by oral gavage (Hazleton Laboratories, 1963a). The animals were observed at 1, 4, and 24 hours post-dosing and then daily for 14 days. One animal died at the 1450 mg/kg dose on day 11. However, no signs of toxicity were observed prior to death and a normal body weight gain was recorded at death. A postmortem examination revealed

congestion of the lungs, kidneys, adrenals, and pancreas, as well as gaseous distention of the stomach and large intestine at the time of death. All other animals showed no gross pathology following termination. Principal toxic effects seen only at the 10,000 mg/kg dose were depression, ataxia, sprawling of limbs and depressed righting reflex only at the 24-hour observation. Based on these results, the acute oral LD_{50} for C6 branched and linear alkyl acetate ester in male Sprague-Dawley rats is >10 g/kg.

An acute oral toxicity study was conducted with C6 branched and linear alkyl acetate ester in accordance with OECD test guideline 401 (EMBSI, 1995b). In this study, 5 male and 5 female Sprague-Dawley rats received 2000 mg/kg of test material as a single dose by oral gavage. The C6 branched and linear alkyl acetate ester did not elicit any signs of acute systemic toxicity. Signs of slight toxicity (staining of the fur and soft stool) were limited to the male animals on Day 0. There was one female death on Day 0, but the death was the result of test material aspiration, not toxicity. Based on these results, the acute oral LD_{50} for C6 branched and linear alkyl acetate ester in rats is >2 g/kg.

Acetic acid, C8-10 branched alkyl esters (CAS RN 108419-33-6)

A GLP compliant acute oral limit study was conducted with C8-C10 branched alkyl acetate ester in Sprague-Dawley rats (BioDynamics, 1983a). In this study, male and female rats (5/sex/dose) received approximately 5.7 ml/kg (i.e., 5.7 g/kg) of test material as a single dose by oral gavage. There was one female death on day 4 during this study. However, all other animals elicited only minimal signs of acute systemic toxicity during the first 4 days of the study, e.g., ano-genital staining, prostration, urinary staining, hypoactivity. All surviving animals showed an increase over pre-dose weights and five of 9 surviving animals showed no observable abnormalities during postmortem examination. Based on these results, the acute LD_{50} for the C8-C10 branched alkyl acetate ester is >5 g/kg.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

In this limit study, 5 male and female Sprague-Dawley rats received 5.7 ml/kg (i.e., 5.7 g/kg) of test material as a single dose by oral gavage (BioDynamics, 1983b). The animals were observed for 14 days. There were no deaths during this study. Signs of slight toxicity were observed only during the first 3 days, i.e., staining of the fur and soft stool. Based on these results, the acute oral LD_{50} for C11-C14 branched alkyl acetate esters in Sprague-Dawley rats is >5 g/kg.

A GLP-compliant repeated-dose probe study was conducted in Sprague-Dawley rats (BioDynamics, 1985b). In this study, 4 male and 4 female rats received 0, 0.1, 0.5, 1.0, or 3.0 g/kg test material by oral gavage once a day for 9 days. With the exception of one animal that was euthanized on Day 7 due to a caging accident, all animals survived to study termination and exhibited increases in body weight. During the course of this study, the administration of C11-C14 branched alkyl acetate esters elicited only minimal signs of acute systemic toxicity. In this study the acute oral LD_{50} was >3 g/kg.

Dermal

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

In this pre-GLP study, white albino rabbits (1/sex/dose) received 50, 200, 794, or 3160 mg/kg of test material in a single dermal application (Hazleton Laboratories, 1963b). The test site was covered with a 24-hour occlusive patch. The animals were observed for 14 days post-dosing. Only three animals exhibited minimal signs of toxicity, i.e., soft feces or diarrhea during this time. There were no gross pathological findings at the study termination and all animals except one exhibited normal body weight gains. The LD_{50} in this study was >3.16 g/kg.

A GLP-compliant acute dermal toxicity study was conducted in New Zealand White rabbits (EMBSI, 1995c). In this study, the rabbits (5/sex/dose) received 2000 mg/kg of test material in a single dermal application. The test site was covered with a 24-hour occlusive patch. The animals

were observed for 14 days post-dosing. No signs of systemic toxicity were observed. Slight dermal irritation was noted in all animals, with the most severe response being observed at the Day 1 observation interval. At post mortem examination, all of the animals had desquamation at the dose site. In general, dermal responses were considered minimal and transient in nature.

In conclusion, the C6 branched and linear alkyl acetate esters did not elicit signs of percutaneous toxicity when administered to intact rabbit skin. The LD_{50} in this study was >2 g/kg.

Acetic acid, C6-8 branched alkyl esters (CAS RN 90438-79-2)

In this study, New Zealand white rabbits (3/sex/dose) received 3160 mg/kg of test material in a single dermal application (BioDynamics Inc., 1983c). The test site was covered with a 24-hour occlusive patch. The animals were observed for 14 days post-dosing. There were no overt signs of systemic toxicity. Clinical observations were made 2, 4, and 24 hours after dosing and on days 3, 7, 10, and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14.

Erythema was noted in all animals at 24 hours, ranging from moderate to severe, and regressed in all animals throughout the study. On Day 14, five or six animals showed very slight erythema and one had no signs of erythema. Edema was evident in all but one animal at 24 hours and by Day 14 all but one animal was free of signs of edema. Desquamation was evident in five animals on Day 14. All animals survived to termination of the study and increased in body weight. There were no significant findings at the postmortem gross examination.

In conclusion, the C6-8 branched alkyl ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin. The LD_{50} in this study was >3.16 g/kg.

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

In this study, New Zealand white rabbits (3/sex/dose) received 3160 mg/kg of test material in a single dermal application (BioDynamics Inc., 1983d). The test site was covered with a 24-hour occlusive patch. The animals were observed for 14 days post-dosing. Clinical observations were made 2, 4, and 24 hours after dosing and on days 3, 7, 10, and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14.

One animal was sacrificed on Day 11 due to severe weight loss. The surviving five animals showed slight weight gain through the study. Dermal evaluations ranged from no erythema to moderate to severe. Edema scores ranged from no edema to slight edema. Desquamation was noted in four animals during the study. The animal terminated on Day 11 revealed kidney discoloration, small spleen, cecum and ileum, and brown material in the stomach. The remaining five animals showed no abnormalities at necropsy.

In summary, the C7-C9 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin. The LD_{50} in this study was >3.16 g/kg.

Acetic acid, C8-10 branched alkyl esters (CAS RN 108419-33-6)

In this study, New Zealand white rabbits (3/sex/dose) received 3160 mg/kg of test material in a single dermal application (BioDynamics Inc., 1983e). The test site was covered with a 24-hour occlusive patch. The animals were observed for 14 days post-dosing. Clinical observations were made 2, 4, and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14.

Erythema was noted in all animals at 24 hours and continued in four animals through Day 14. Edema was seen in three animals at 24 hours. No animals showed edema by the Day 7 evaluation. Desquamation was seen in one animal on Day 7, three animals on day 10 and remained in two

animals at the Day 14 termination. One male and two females at Day 7 showed slight decreases in body weight. Food consumption was reduced on Day 1 only. Postmortem examination revealed gallbladder and salivary gland abnormalities, kidney discoloration, a urinary bladder abnormality, hair in two stomachs and ano-genital staining.

In conclusion, C8-C10 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin. The LD_{50} for this study was >3.16 g/kg.

Acetic acid, C9-11 branched alkyl esters (CAS RN 108419-34-7)

In this study, New Zealand white rabbits (3/sex/dose) received 3160 mg/kg of test material in a single dermal application (BioDynamics Inc., 1984a). The test site was covered with a 24-hour occlusive patch. The animals were observed for 14 days post-dosing. Clinical observations were made 2, 4, and 24 hours after dosing and on days 3, 7, 10, and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14.

There were no deaths during the course of this study. Three of six animals gained weight during the study. Clinical in-life observations included ano-genital staining, ocular discharge, unthrifty coat, nasal discharge and poor food consumption. Erythema and edema were slight to well defined. Desquamation was also observed. Postmortem examination revealed kidney discoloration an encapsulated salivary gland, an enlarged cervical lymph node and hair present in the stomach.

In summary, C9-C11 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in single dose to intact rabbit skin. The LD_{50} in this study is >3.16 g/kg.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

In this study, New Zealand White rabbits (3/sex/dose), received 3160 mg/kg of test material in a single dermal application (BioDynamics Inc., 1984b). The test site was covered with a 24-hour occlusive patch. The animals were observed for 14 days post-dosing. There were no overt signs of systemic toxicity. At day 7, five of six rabbits exhibited slight body weight decreases. However, only 2 animals continued to have decreased body weight at day 14. Overall, dermal responses were considered minimal and transient in nature.

In conclusion, the C11-C14 branched alkyl acetate esters did not elicit signs of percutaneous toxicity when administered to intact rabbit skin. The LC_{50} in this study was >3.16 g/kg.

3.1.3 Irritation

Skin Irritation

Studies in Animals

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

A primary dermal irritation study was conducted with C6 branched and linear alkyl acetate ester in accordance with OECD test guideline 404 (EMBSI, 1995d). In this study, a single dermal application of test material (0.5 ml) was applied to 6 New Zealand White male rabbits. The test site was covered with a 4-hour semi-occlusive patch. The animals were observed and scored for erythema and edema at 1, 24, 48, and 72 hours and 7 days post dosing.

All animals survived to study termination, were free of clinical signs, and displayed an increase in body weight during the test period. All of the animals displayed erythema and edema in the first 72 hours. The mean scores were 1.72 (erythema) and 1.17 (edema). All of the animals were free of erythema and edema at the Day 7 observation period and the study was terminated. The Primary Irritation Index (PII) for this study was 3.08.

Based on these results, the C6 branched and linear alkyl acetate ester is considered to be a moderate dermal irritant to rabbit skin.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

A primary dermal irritation study was conducted with C11-C14 branched alkyl acetate ester in accordance with EPA test guideline 798.4470 (BioDynamics Inc., 1983f). In this study, a single dermal application of test material (0.5 ml) was applied to New Zealand White rabbits (3/sex/dose). The test site was covered with a 4-hour semi-occlusive patch. The animals were observed and scored for erythema and edema at 1, 24, 48, and 72 hours and 7 days post dosing.

All animals survived to study termination, were free of clinical signs, and 5 of 6 animals displayed an increase in body weight during the test period. All of the animals displayed erythema in the first 72 hours. The mean score for erythema was 0.67. One of 6 animals showed very slight erythema at the Day 7 observation point. The Primary Irritation Index (PII) for this study was 0.67.

Based on these results, the C11-C14 branched alkyl acetate ester is considered to be a mild dermal irritant to rabbit skin.

Eye Irritation

Studies in Animals

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

C6 branched and linear alkyl acetate ester was tested in a Draize Ocular Irritation study (Hazleton Laboratories, 1963c). In this pre-GLP study, 0.1 ml of test material was instilled into the conjunctival sac of the left eye of 6 albino rabbits. The rights eye of each rabbit was left untreated and served as the control. The animals were observed at 1, 4 and 24 hours post-dosing and again at 2, 3, 4, and 7 days.

Ocular irritation was most prominent at the 1-hour observation point when the total Draize scores ranged from 8 to 12 (Maximum possible score = 110). Irritation was confined to the conjunctivae and generally consisted of moderate redness, chemosis and discharge. The signs of eye irritation completely subsided in all animals by day 7. Fluorescein examination on day 7 confirmed the absence of any corneal damage.

Based on these results (i.e., Draize Score = 12), the C6 branched and linear alkyl acetate ester was considered to be a mild reversible irritant causing minimal irritation.

C6 branched and linear alkyl acetate ester was tested in a Draize Ocular Irritation study in accordance with OECD test guideline 405 (EMBSI, 1995e). In this study, 0.1 ml of test material was instilled into the conjunctival sac of the left eye of 6 male New Zealand White rabbits. The rights eye of each rabbit was left untreated and served as the control. The animals were observed at 1, 4 and 24 hours post-dosing.

Ocular irritation was most prominent at the 1-hour observation point when the total Draize scores ranged from 10 to 12 (Maximum possible score = 110). Irritation was confined to the conjunctivae and generally consisted of redness, chemosis and discharge. The signs of eye irritation completely subsided in all animals by the 72-hour evaluation point. Fluorescein examination at 72 hours confirmed the absence of any corneal damage.

Based on these results (i.e., Draize Score = 12), the C6 branched and linear alkyl acetate ester was considered to be a mild reversible irritant.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

C11-C14 branched alkyl acetate ester was tested in a Draize Ocular Irritation study (BioDynamics Inc., 1983g). In this study, 0.1 ml of test material was instilled into the conjunctival sac of the right eye of New Zealand White rabbits (3/sex/dose). The left eye of each rabbit was left untreated and

served as the control. The animals were observed at 1, 4, 24, 48, and 72-hours post-instillation and again on days 4 and 7.

Ocular irritation was most prominent at the 1-hour observation point when the total Draize scores ranged from 0 to 6 (Maximum possible score = 110). Irritation was confined to the conjunctivae and generally consisted of redness, chemosis and discharge. Corneal ulceration was noted and confirmed using rluorescein stain in one animal at the 24-hour observation. The signs of eye irritation completely subsided in all animals by day 7.

Based on these results the C11-C14 branched alkyl acetate ester was considered to be a mild reversible irritant.

3.1.4 Sensitization

Skin

Studies in Humans

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

A repeated insult patch test was conducted in human volunteers with hexanol, acetate, branched and linear (Hilltop Research, Inc., 1991). This study was conducted in order to evaluate whether repetitive application of this material to the skin of human volunteers would induce contact sensitization. The experimental design used for this study was an adaptation of the Draize Patch Test (Draize, 1959). In this study, the hexanol, acetate, branched and linear did not produce any evidence of skin sensitization.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

A repeated insult patch test was conducted in human volunteers with acetic acid, C11-14 branched alkyl ester (Hilltop Research, Inc., 1991). This study was conducted in order to evaluate whether repetitive application of this material to the skin of human volunteers would induce contact sensitization. The experimental design used for this study was an adaptation of the Draize Patch Test (Draize, 1959). In this study, the acetic acid, C11-14 branched alkyl ester did not produce any evidence of skin sensitization.

3.1.5 Repeated Dose Toxicity Studies in Animals

Oral

Studies in Animals

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

A repeated dose oral toxicity study was conducted with C6 branched and linear alkyl acetate ester in Crl:CD BR rats in accordance with OECD test guideline 407 (EMBSI, 1995f). In this study, the rats (5/sex/dose) received 0, 100, 500, and 1000 mg/kg of test material per day for 28 days by oral gavage. No signs of overt systemic toxicity were observed at any dose level. During the study, no adverse effects on body weight, food consumption, clinical laboratory parameters or organ weights were observed. In addition, all clinical in-life, gross postmortem and microscopic findings were normal.

In conclusion, repeated oral administration of C6 branched and linear alkyl acetate ester to rats for 28 days did not produce any adverse effects at any dose level tested. The No Observed Adverse Effect Level (NOAEL) in this study was 1.0 g/kg/day.

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

In this oral repeated dose study, Sprague-Dawley rats (20/sex/dose) received 0, 0.1, 0.5, and 1.0 g/kg of test material by gavage, 5 days/week for 13 weeks (BioDynamics Inc., 1985c). During this study only minimal signs of toxicity were observed and there was no treatment-related mortality. The in-life clinical observations consisted primarily of oral and dermal irritation. However, there was no clear dose-response. The weekly mean body weights and food consumption values were not significantly altered compared to controls. In addition, the qualitative hematologic data were unremarkable at all dose levels for the interim and terminal evaluations. At the terminal sacrifice, there were no biologically significant differences between treated and control animals for the measured clinical chemistries. Although terminal liver and kidney weights were elevated in a dose-related manner, they were considered to be adaptive changes and not indicative of toxic effects. All other organ weights were comparable to control values. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy only in the high-dose male rats that is consistent with alpha-2-μ-globulin effects. This effect is known to be male rat specific and is not relevant for humans. Histopathology review of all other tissues from high-dose animals, including reproductive organs showed normal morphology. Based on these results, the No Observed Adverse Effect Level (NOAEL) for C7-C9 branched alkyl acetate esters in this study is 1.0 g/kg/day.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

In this oral repeated dose study, Sprague-Dawley rats (20/sex/dose) received 0, 0.1, 0.5, and 1.0 g/kg of test material by gavage, 5 days/week for 13 weeks (BioDynamics Inc., 1985d). During this study only minimal signs of toxicity were observed and there was no treatment-related mortality. The in-life clinical observations consisted primarily of oral and dermal irritation. However, there was no clear dose-response. The weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels. Terminal liver and kidney weights were elevated in a dose-related manner but these were considered to be adaptive changes and not indicative of toxicity. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy in the mid- and high-dose male rats that is consistent with alpha-2-μ-globulin effects. This effect is known to be male rat specific and is not relevant for humans. Histopathology review or all other tissues from high-dose animals including reproductive organs showed normal morphology. Based on these results, the No Observed Adverse Effect Level (NOAEL) for C11-C14 branched alkyl acetate esters in this study is 1.0 g/kg/day.

3.16 Mutagenicity

In vitro Studies

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

C6 branched and linear alkyl acetate ester was tested in an Ames Assay in 5 strains of *Salmonella typhimurium* (i.e., TA98, TA100, TA1535, TA1537 and TA1538) with and without metabolic activation (EMBSI, 1995g). Each of the five strains was dosed with 250, 500, 1000, 2000, and 3000 μg/plate of test substance; a vehicle control (DMSO); a non-treated control and a positive control. There were 3 plates/dose group/strain/treatment set.

The C6 branched and linear alkyl acetate ester did not induce significant increases in revertant colonies (≥3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. Toxicity was observed in both the initial and repeat assays in all strains at one or more dose levels with and/or without metabolic activation. The non-treated and vehicle controls responded in a manner consistent with data from previous assays.

In conclusion, the C6 branched and linear alkyl acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested, but was toxic in all strains tested under the conditions of this study.

C6 branched and linear alkyl acetate ester was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation (EMBSI, 1995h). A repeat assay was also performed using 20-hour and 44-hour harvests. Treatment group doses (14 total in initial and repeat assays) ranged from 250-480 μg/mL in the 20-hour initial test; 230-550 μg/mL in the 20- and 44-hour repeat assays. DMSO was used as the vehicle. Positive controls included N-methyl-N-Nitro-N-Nitrosoguanidine (NMNG), a direct acting clastogen which does not require metabolic activation and 7,12-dimethylbenz(a)anthracene (DMBA), a clastogen that does require metabolic activation.

In the initial 20-hour harvest data, there was no evidence of a positive dose response nor of any treated group being different from the control in these analyses. For the repeat harvest, the high dose group was statistically different from the vehicle control. However, this statistically significant finding was not reproducible. No increase was observed at the 44-hour harvest time. In addition, no increase was observed in the initial assay with metabolic activation at similar dose levels. There was no statistically significant finding in the 44-hour harvest.

The C6 branched and linear alkyl acetate ester reduced survival by at least 50% when compared to the vehicle control in the repeat assay: 20-hour harvest without activation and 44-hour harvest with and without metabolic activation. All negative and positive controls used in this study performed in an appropriate. Based on these results, the C6 branched and linear alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 550 μg/mL with and 430 μg/mL without metabolic activation.

Acetic acid, C6-8 branched alkyl esters (CAS RN 90438-79-2)

C6-C8 branched alkyl acetate ester was tested in an Ames Assay in 5 strains of *Salmonella typhimurium* (i.e., TA98, TA100, TA1535, TA1537, and TA1538) with and without metabolic activation (EMBSI, 1997b). Each of the five strains was dosed with 50, 100, 200, 400, 600, and 800 μg/plate of test substance (50 during repeat assay only; 800 during initial assay only); a vehicle control (DMSO); a non-treated control and a positive control. There were 3 plates/dose group/strain/treatment set.

The C6-C8 branched alkyl acetate ester did not induce significant increases in revertant colonies (i.e., >3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. Toxicity was observed in both the initial and repeat assays in most strains at one or more dose levels with and/or without metabolic activation. The non-treated and vehicle controls responded in a manner consistent with data from previous assays.

In summary, the C6-C8 branched alkyl acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested, even at doses that produced evidence of toxicity.

C6-C8 branched alkyl acetate ester was also tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation (EMBSI, 1997c). A repeat assay was also performed using 20-hour and 44-hour harvests. Treatment group doses (11 total in initial and repeat assays) ranged from 80-240 mg/mL in the 20-hour initial test; 40-200 mg/mL in the 20- and 44-hour repeat assays. DMSO was used as the vehicle. N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - a clastogen that does not require metabolic activation) and 7,12-dimethylbenz(a)anthracene (DMBA - clastogen that requires metabolic activation) were used as positive controls in the non-activated series and activated series, respectively.

For the initial 20-hour harvest data, there was a notable decrease in the percent cell confluency at concentrations ≥180 mg/mL with activation and at concentrations ≥140 mg/mL without activation. Cell morphology and mitotic indices were acceptable at or below these levels and cell death was prevalent above these levels. For the repeat assay, there were no statistically significant dose-related trends in the percentage of aberrant cells and none of the test concentrations were statistically different than the vehicle control in the 20 or 44 hour activated or non-activated series. The percentage of aberrant cells in the vehicle control groups ranged from 1% to 2.0%, and the percentage of aberrant cells in the treated groups ranged from 0.0% to 2.6% for the 20 and 44 hour activated and non-activated series. All negative and positive controls used in this study performed in an appropriate manner.

In conclusion, the C6-C8 branched alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 180 mg/mL with and 140 mg/mL without metabolic activation.

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

C7-C9 branched alkyl acetate ester was tested in an Ames Assay in 5 strains of *Salmonella typhimurium* (i.e., TA98, TA100, TA1535, TA1537, and TA1538) with and without metabolic activation (EMBSI, 1994b). Each of the five strains was dosed with 25, 50, 100, 200, 400, and 600 µg/plate of test substance (25 during repeat assay only; 600 during initial assay only); a vehicle control (DMSO); a non-treated control and a positive control:

C7-C9 branched alkyl acetate ester did not induce significant increases in revertant colonies (>3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was observed for all five tester strains with and without metabolic activation in both the initial and repeat assays, except for tester strain TA1535 with metabolic activation for the repeat assay. The non-treated and vehicle controls responded in a manner consistent with data from previous assays.

In conclusion, C7-C9 branched alkyl acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

C11-C14 branched alkyl acetate ester was tested in an Ames Assay in 5 strains of *Salmonella typhimurium* (i.e., TA98, TA100, TA1535, TA1537, and TA1538) with and without metabolic activation (EMBSI, 1994c). Each of the five strains was dosed with 156, 312.5, 625, 1250, 2500, 5000, and 10,000 µg/plate of test substance; a vehicle control (DMSO); a non-treated control and a positive control. There were 3 plates/dose group/strain/treatment set.

The C11-C14 branched alkyl acetate ester, did not induce significant increases in revertant colonies (≥ 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was not observed. Test substance beading was observed for all tester strains, both with and without metabolic activation at 1250 through 10,000 ug/plate. The non-treated and vehicle controls responded in a manner consistent with data from previous assays.

In conclusion, the C11-C14 branched alkyl acetate ester was not mutagenic in any strain of *Salmonella typhimurium* tested, and was not toxic in any strain tested under the conditions of this study.

In vivo Studies

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

An *in vivo* mammalian bone marrow micronucleus assay was conducted in male and female CD-1 mice with C7-C9 branched alkyl acetate esters (EMBSI, 1994d). In this study, the test material was administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control, i.e., cyclophosphamide, was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two-slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for the presence of micronuclei. 1000 polychromatic erythrocytes per animal, were evaluated.

A statistically significant increase in the mean number of micronucleated polychromatic erythrocytes was not seen at any dose level. Cytotoxicity, shown by a dose-related decrease in the percentage of polychromatic erythrocytes, was observed for both sexes at the 48-hour sampling time (regression coefficient $p<0.01$). The two highest dose groups were statistically different from the vehicle control. Both the positive (cyclophophamide) and negative (vehicle carrier) controls responded in an appropriate manner. The test material is considered to be toxic to bone marrow in CD-1 mice under the conditions of this test based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

Under the conditions of this study, C7-C9 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

C11-C14 branched alkyl acetate ester was evaluated *in vivo* for its ability to induce micronuclei in bone marrow polychromatic erythrocytes (PCEs) in male and female Crl:CD-1 (VAF/Plus) mice (EMBSI, 1994e). Five mice/sex/dose were used. In this study, 0.45, 0.90, and 1.8 grams/kg of test material was administered as a single dose by oral gavage. The vehicle, i.e., corn oil and positive control, i.e., cyclophosphamide, were also administered by oral gavage at a volume equal to the volume of the test material. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with the positive control, cyclophosphamide, were sacrificed at 24 hour only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animals were made. The slides were stained and then evaluated for the presence of micronuclei (1000 polychromatic erythrocytes/animal were evaluated).

A dose-related decrease in the percentage of polychromatic erythrocytes was observed for the female 48-hour sampling time. However, none of the dose groups were statistically different from the control. The positive control induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes which indicates that the positive control is clastogenic and is responding in an appropriate manner. Vehicle carrier control values for the mean percent of polychromatic erythrocytes and for the mean percent of micronucleated polychromatic erythrocytes responded in an appropriate manner.

Under the conditions of this assay, the C11-C14 branched alkyl acetate ester is considered to be toxic to bone marrow in CD-1 mice based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time. However, it did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.

3.1.6 Carcinogenicity

No data are available.

3.1.7 Toxicity for Reproduction

Studies in Animals

Developmental Toxicity

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

A developmental toxicity study was conducted in female Sprague-Dawley rats in accordance with EPA Test Guideline 798.4900 (BioDynamics Inc., 1985e). In this study, 22 mated female rats received 0, 100, 500, and 1000 mg/kg C7-C9 branched alkyl acetate ester daily by oral gavage on days 6-15 of gestation.

Maternal toxicity was observed at the 500 and 1000 mg/kg doses as evidenced by decreases in body weight and food consumption. However, slight increases in fetal malformations and embryotoxicity were only observed in the high dose group, i.e., 1000 mg/kg. No adverse fetal effects were observed in the 100 and 500 mg/kg dose groups.

In conclusion, C7-C9 branched alkyl acetate ester should not be considered as a selective developmental toxicant as fetal malformations were only observed at the highest maternally toxic dose, i.e., 1000 mg/kg.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

A developmental toxicity study was conducted in female Sprague-Dawley rats in accordance with EPA Test Guideline 798.4900 (BioDynamics Inc., 1985f). In this study, 22 mated female rats received 0, 500, 1300, and 2500 mg/kg C11-C14 branched alkyl acetate ester daily by oral gavage on days 6-15 of gestation.

Maternal toxicity was observed at the 1300 and 2500 mg/kg doses as evidenced by decreases in body weight. There were no statistically significant deleterious effects on fetal survival, body weight, or crown-rump length and no evidence of treatment-related malformations.

In conclusion, C11-C14 branched alkyl acetate ester is not a selective developmental toxicant.

3.2 Initial Assessment for Human Health

Members of the Alkyl Acetate C6 to C13 Category have a low order of toxicity by the oral and dermal routes of exposure. Oral LD_{50}s range from >2000 to 10,000 mg/kg and dermal LD_{50}s range from >2000 to 3160 mg/kg. Thus, the acute oral and dermal toxicity for the Alkyl Acetate C6 to C13 Category is well characterized.

Studies have demonstrated that the members of the Alkyl Acetate C6 to C13 Category are mildly to moderately irritating to the skin and only mildly irritating to the eyes. Thus, the skin and eye irritation potential for the Alkyl Acetate C6 to C13 Category has been well characterized and no further studies are proposed.

Members of the Alkyl Acetate C6 to C13 Category are not expected to be skin sensitizers in animals or humans as a structurally similar chemical, 1-hexanol, did not induce sensitizing reactions in guinea pigs or humans. Data are not available to assess the potential for respiratory tract sensitization in animals or humans. However, since the members of this category are not expected to be skin sensitizes, they are also not expected to be respiratory tract sensitizes. Additionally, due to the low to moderate vapour pressure of members of this category, potential atmospheric exposure is expected to be limited.

A repeated dose oral toxicity study was conducted with C6 branched and linear alkyl acetate ester in rats. In this study, the rats received 0, 100, 500, and 1000 mg/kg of test material per day for 28 days by oral gavage. The repeated oral administration of C6 branched and linear alkyl acetate ester to rats for 28 days did not produce any adverse effects at any dose level tested. The No Observed Adverse Effect Level (NOAEL) in this study was 1000 mg/kg/day. Repeated dose oral toxicity studies were also conducted with C7-C9 and C11-C14 branched alkyl acetate esters. In these studies, rats received 0, 100, 500, and 1000 mg/kg of test material by oral gavage, 5 days/week for 13 weeks. No significant treatment-related effects were observed during these studies. Although terminal liver and kidney weights were elevated in a dose-related manner, they were considered to be adaptive changes and not indicative of toxic effects. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy only in high dose male rats in both studies. This is consistent with alpha-2-μ-globulin effects. This effect is known to be male rat specific and is not relevant for humans. Histopathology of all other tissues from high dose animals showed normal morphology. Based on these results, the No Observed Adverse Effect Level for C7-C9 and C11-C14 branched alkyl acetate esters is 1000 mg/kg/day. In summary, based on the results of the repeated-dose studies conducted in animals, the members of the Alkyl Acetate C6 to C13 Category appear to have a low order of subchronic toxicity.

Members of the Alkyl Acetate C6 to C13 Category appear to have a low potential for mutagenic effects. C6 branched and linear alkyl acetate, C6-C8 branched alkyl acetate ester, C7-C9 branched alkyl acetate, and C11-C14 branched alkyl acetate ester were all tested in an Ames Assay in 5 strains of *Salmonella typhimurium* either in the presence or absence of metabolic activation. None of the materials tested were mutagenic in any of the *Salmonella* strains tested. In addition, C6 branched and linear alkyl acetate and C6-C8 branched alkyl acetate ester were tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. Both materials were considered to be negative for inducing chromosome aberrations under the conditions of the assay. *In vivo* mammalian bone marrow micronucleus assays were also conducted in CD-1 mice with C7-C9 branched alkyl ester and C11-C14 branched alkyl acetate ester. Neither material induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Thus, both materials were considered to be non-mutagenic under the conditions of this assay. Based on the above data, the mutagenic potential for the Alkyl Acetate C6 to C13 Category has been well characterized. By read-across, these data also support characterizing the untested members of this category as having a low potential for carcinogenicity.

Developmental toxicity studies were conducted in female Sprague-Dawley rats by the oral route of exposure with C7-C9 and C11-C14 branched alkyl acetate esters. Exposure of rats to the C7-C9 branched alkyl acetate ester resulted in slight increases in fetal malformations and embryotoxicity at the highest dose tested, i.e., 1000 mg/kg. However, as this dose produced maternal toxicity, the C7-C9 branched alkyl acetate ester should not be considered as a selective developmental toxicant. Exposure of rats to the C11-C14 branched alkyl esters produced maternal toxicity at the two highest doses tested, 1300 and 2500 mg/kg. However, there were no statistically significant deleterious effects on fetal survival, body weight, or crown-rump length and no evidence of treatment-related malformations. Thus, the C11-C14 branched alkyl acetate ester is not a selective developmental

toxicant. Based on these results, the members of the Alkyl Acetate C6 to C13 Category appear to have a low order of developmental toxicity.

In conclusion, members of the Alkyl Acetate C6 to C13 Category have a low order of acute toxicity, are mild to moderate skin irritants, are mild reversible eye irritants and are not expected to produce skin or respiratory tract sensitization. Subchronic studies have also shown a low order of toxicity. The only effect observed upon microscopic evaluation in these studies was evidence of mild tubular nephropathy in the high-dose males. This effect is known to be male rat specific and is not relevant for humans. Testing in a variety of *in vitro* and *in vivo* genotoxicity assays has not shown any mutagenic activity with or without metabolic activation. Based on these negative genotoxicity data, category members are expected to have a low potential for carcinogenicity. Reproductive/ developmental testing has shown fetal effects in some studies, but only at doses that produced overt maternal toxicity. Thus, these data support that members of this category are not selective reproductive toxicants. Taken in concert, these data show that the toxicity of members in the Alkyl Acetate C6 to C13 Category, for the endpoints discussed, has been well characterized and support an overall low hazard assessment for category members.

4 HAZARDS TO THE ENVIRONMENT

4.1 Aquatic Effects

Acute Toxicity Test Results

Hexanol, acetate, branched and linear (CAS RN 88230-35-7)

The acute toxicity of hexanol, acetate, branched and linear was investigated with a freshwater fish (*Oncorhynchus mykiss*) following OECD 203 test guidelines. The study was conducted using static-renewal procedures with approximately 80% of the test solution in each test replicate renewed at 24-hour intervals. Individual Water Accommodated Fractions (WAF) were mixed at nominal levels of 0, 0.5, 1.3, 3.2, 8.0, and 20 mg/L. The 96-hour LL_{50} was 11.9 mg/L (EMBSI, 1995i).

Hexanol, acetate, branched and linear was also investigated for its effects on the freshwater invertebrate (*Daphnia magna*) following OECD 202 test guidelines. Individual WAFs were mixed at nominal levels of 0, 0.1, 0.5, 1.0, 5.0, and 10 mg/L. Under static conditions, the study reported a 48-hour EL_{50} of 7.6 mg/L (EMBSI, 1995j).

An acute experimental value is also reported for a freshwater green alga (*Pseudokirchneriella subcapitata*). Hexanol, acetate, branched and linear was tested following OECD 201 test guidelines. Individual WAFs were prepared at nominal levels of 0, 8, 31, 62, 125, and 250 mg/L in algal nutrient media. Each test replicate was inoculated with 1.0×10^4 algal cells/mL and placed on an oscillating table under continuous lighting. Under static conditions, the 96-hour EL_{50} values based on biomass and growth rate were 40.1 and 32.1 mg/L, respectively, with corresponding No Observed Effect Level (NOEL) values of 31.0 and 8.0 mg/L, respectively (EMBSI, 1995k).

Acetic acid, C6-8 branched alkyl esters (CAS RN 90438-79-2)

The acute toxicity of Acetic acid, C6-8 branched alkyl esters was investigated with a freshwater fish (*Oncorhynchus mykiss*) following OECD 203 test guidelines. The study was conducted using static-renewal procedures with approximately 80% of the test solution in each test replicate renewed at 24-hour intervals. Individual Water Accommodated Fractions (WAF) were mixed at nominal levels of 0, 2, 4.5, 10, 23, and 50 mg/L. Corresponding measured values based on GC-FID analysis were 0, 1.2, 1.59, 5.39, 21.1, and 43.6 mg/L. The 96-hour LC_{50} was 8.18 mg/L (EMBSI, 1997d).

Acetic acid, C7-9 branched alkyl esters (CAS RN 108419-32-5)

The acute toxicity of Acetic acid, C7-9 branched alkyl esters was investigated with a freshwater fish (*Pimephales promelas*) following USEPA TSCA Environmental Effects test guidelines. The study was conducted under flow-through conditions. A stock WAF was prepared by adding 267 ml of the test substance to 40 L of dilution water. The 100% WAF stock was delivered to the test chambers via a diluter system where it prepared test treatments at nominal levels of 0, 4.4, 8.8, 17.5, 35, and 70% WAF, which measured 0, 1.39, 2.71, 4.90, 9.91, and 19.86 mg/L as Total Carbon (TC). The 96-hour LC_{50} was 14.9 mg/L based on TC (BioDynamics, 1985g).

Acetic acid, C7-9 branched alkyl esters was also investigated for its effects on the freshwater invertebrate (*Daphnia magna*) following USEPA 560/6-82-002 Environmental Effects test guidelines. The study was conducted under flow-through conditions. A stock WAF was prepared by combining Acetic acid, C7-9 branched alkyl esters with dilution water at a ratio of 6.7 ml per liter of water. The 100% WAF stock was delivered to the test chambers via a diluter system where it prepared test treatments at nominal levels of 0, 6.25, 12.5, 25, 50, and 100% WAF, which measured 0, 1.87, 4.13, 10.24, 20.21, and 39.95 mg/L as Total Carbon (TC). The 48-hour EC_{50} was 29.4 mg/L based on TC (BioDynamics, 1985h).

Acetic acid, C9-11 branched alkyl esters (CAS RN 108419-34-7)

Acetic acid, C9-11 branched alkyl esters was investigated for its effects on the freshwater invertebrate (*Daphnia magna*) following OECD 202 test guidelines. Individual WAFs were prepared at nominal levels of 0, 1.3, 3.2, 8, 20, and 50 mg/L. Under static conditions, the study reported a 48-hour EL_{50} of 6.7 mg/L (EMBSI, 2000).

An acute toxicity test was proposed and conducted using the freshwater green alga (*Pseudokirchneriella subcapitata*) following OECD 201 test guidelines (EMBSI, 2003). Individual treatments were prepared as WAFs at nominal levels of 0, 64.5, 130, 254, 522, and 1021 mg/L in algal nutrient media. Each test replicate was inoculated with 1.0×10^4 algal cells/mL at the start of the study and placed on an oscillating table under continuous lighting. Under static conditions, the 72-hour EC_{50} values for biomass and growth rate were both >1021 mg/L. The corresponding NOEL values for biomass and growth rate were both 254 mg/L. Results of this study were reported based on the nominal loading levels.

Acetic acid, C11-14 branched alkyl esters (CAS RN 108419-35-8)

The acute toxicity of Acetic acid, C11-14 branched alkyl esters was investigated (BioDynamics, 1985i) with a freshwater fish (*Pimephales promelas*) following USEPA TSCA Environmental Effects test guidelines (USEPA 40 CFR 792). The study was conducted under flow-through conditions. A stock WAF was prepared at a ratio of 1:150 of the test substance to dilution water, the result was designated as 100% WAF. The 100% WAF stock was delivered to the test chambers via a diluter system where it prepared test treatments at nominal levels of 0, 6.25, 12.5, 25, 50, and 100% WAF. No mortality was observed during the study, which reported a 96-hour LL_0 of 5800 mg/L (calculated based on nominal loading levels).

Acetic acid, C11-14 branched alkyl esters was also investigated for its effects on the freshwater invertebrate (*Daphnia magna*) following USEPA 560/6-82-002 Environmental Effects test guidelines. The study was conducted under static conditions. A stock WAF was prepared by combining Acetic acid, C7-9 branched alkyl esters with dilution water at a ratio of 6.7 ml per liter of water. The 100% WAF stock was diluted to prepare test treatments at nominal levels of 0, 6.25, 12.5, 25, 50, and 100% WAF. No immobilization was observed during the study, which reported a 48-hour EL_0 of 5829 mg/L (calculated based on nominal loading levels)(BioDynamics, 1985j).

An acute toxicity value is reported for the freshwater green alga (*Pseudokirchneriella subcapitata* formerly *Selenastrum capricornutum*) (BioDynamics, 1985k). Acetic acid, C11-14 branched alkyl esters was tested following methods described in USEPA Environmental Effects test guidelines (EPA 560/6-83-002). A stock WAF was prepared and then divided into test treatments at nominal

levels of 0, 6.25, 12.5, 25, 50, and 100% WAF. Each replicate chamber was inoculated with 2.0 x 10^4 algal cells/mL at the start of the study and placed on an oscillating table under continuous lighting. Under static conditions, the 96-hour EL_0 values for both biomass and growth rate were 5829 mg/L. The corresponding NOEL value was 5829 mg/L for both biomass and growth rate (calculated based on nominal loading levels.

4.2 Terrestrial Effects

There are no experimental data available using standard testing procedures that can be used to assess the terrestrial hazard of members of the Alkyl Acetate C6 to C13 Category.

4.3 Initial Assessment for the Environment

In spite of their low to moderate vapour pressure, results of distribution modelling show that category members will partition predominantly to the air compartment, with the exception of acetic acid, C11-14 branched alkyl esters, which is expected to partition predominantly to the soil compartment. The air compartment is a primary compartment for these substances because the partitioning results are based on the chemical being at equilibrium, which does not show the period of time to reach this state. These results do suggest that assessment of these substances should not overlook their fate in the air where they have the potential to partition. Volatilization to the air from aqueous and terrestrial habitats is expected to occur at appreciable rates for most of these substances, and once in the air, they have the potential to rapidly degrade through indirect photolytic processes mediated primarily by hydroxyl radicals. This can be a significant route of loss and therefore a significant degradation process for members of this category. Aqueous photolysis and hydrolysis will not contribute to the transformation of category constituents in aquatic environments because they are either poorly or not susceptible to these reactions.

Biodegradability of the alkyl acetates has been evaluated with standard 28-day test guidelines. The results from these studies show that the alkyl acetates are subject to microbial degradation under aerobic conditions and that all but the C11-C14 branched alkyl acetate ester are expected to biodegrade at rapid rates, greater than 77% in 28 days.

Member substances of the Alkyl Acetate C6 to C13 Category have been shown to exhibit low to moderate acute aquatic toxicity. This assessment is supported by the results of aquatic toxicity studies for several organisms. Members ranging from the C6 branched and linear alkyl acetate ester to the C9-C11 branched alkyl acetate ester are expected to produce a relatively narrow range of moderate acute toxicity to freshwater aquatic organisms in the range of 7 to 40 mg/L. In comparison, the C11-C14 branched alkyl acetate is not expected to produce acute aquatic toxicity to freshwater fish and invertebrates, or toxicity to freshwater algae, based on results of studies for this substance. The lack of toxicity is due to its comparatively lower water solubility, which limits the exposure of aquatic organisms to soluble fractions of this substance.

Category members have a low potential to bioaccumulate in aquatic species based on a calculated bioconcentration factor range of 30 to 754 (log BCF = 1.5 to 2.9).

Category members are expected to be removed in wastewater treatment facilities. A predominant mechanism accounting for their removal is biodegradation, followed with partitioning or sorbtion to sludge solids contributing to the remaining loss.

5 DATA SUMMARY

Physico-chemical, environmental fate and effects, and human health data that characterize the 6 substances in the Alkyl Acetate C6 to C13 Category are summarized in Tables 7 and 8.

Table 7. Summarized Physico-Chemical and Environmental Data for Members in the Alkyl Acetate C6 to C13 Category

Endpoint	Hexanol, acetate branched and linear alkyl esters (C6-rich)	Acetic acid, C6-8, branched alkyl esters (C7-rich)	Acetic acid, C7-9, branched alkyl esters (C8-rich)	Acetic acid, C8-10, branched alkyl esters (C9-rich)	Acetic acid, C9-11, branched alkyl esters (C10-rich)	Acetic acid, C11-14, branched alkyl esters (C13-rich)
	88230-35-7	90438-79-2	108419-32-5	108419-33-6	108419-34-7	108419-35-8
Melting Point (°C)	-59	-50	-30	-20	-8.8	-2
Boiling Range (°C)	164 to 176	176 to 200	186 to 215	205 to 235	220 to 250	240 to 285
Vapor Pressure (hPa)	1.93	0.68	0.93	0.35	0.13	0.01
Log K_{ow}	2.83	3.32	3.66	4.15	4.65	6.05
Water Solubility (mg/L)	309	102	45	14.5	4.7	0.2
Direct Photodegradation	Direct photolysis will not contribute to degradation					
Indirect (OH-) Photodegradation* (half-life, hrs)	17.3	14.5	12.5	10.5	9.3	6.9
Hydrolysis	Hydrolysis will not contribute to degradation					
Distribution	Predominantly in air compartment					Predominantly in soil compartment

* Atmospheric half-life values are based on a 12-hr day.

Table 7. Continued

Endpoint	Hexanol, acetate branched and linear alkyl esters (C6-rich)	Acetic acid, C6-8, branched alkyl esters (C7-rich)	Acetic acid, C7-9, branched alkyl esters (C8-rich)	Acetic acid, C8-10, branched alkyl esters (C9-rich)	Acetic acid, C9-11, branched alkyl esters (C10-rich)	Acetic acid, C11-14, branched alkyl esters (C13-rich)
	88230-35-7	90438-79-2	108419-32-5	108419-33-6	108419-34-7	108419-35-8
Percent Biodegradation, after 28 days (unacclimated inoculum)	76.9	77.1	77.1 to 84.7 (ra)		84.7	31.0 (acclimated inoculum)
Bioconcentration Factor (log value)	30 (1.5)	63 (1.8)	151 (2.2)	316 (2.5)	754 (2.9)	325 (2.5)
96-hr Fish LC_{50}, mg/L	11.9 (n)	8.2 (m)	14.9 (m)	14.9 (m, ra)		nes
48-hr Invertebrate EC_{50}, mg/L	7.6 (n)	7.6 (n, ra)	29.4 (m)	6.7 (n, ra)	6.7 (n)	nes
96-hr Alga EC_{50}, mg/L	32.1 r (n) 40.1 b (n)	32.1 r (n, ra) 40.1 b (n, ra)			>1021 r/b (n) *	nes
96-hr Alga NOEC, mg/L	8.0 r (n) 31.0 b (n)	8.0 r (n, ra) 31.0 b (n, ra)			254 r/b (n)**	5829 r/b (n) nes

(ra) read-across data
(n) nominal
(m) measured
nes no effect at saturation
b biomass
r growth rate
* 72-hour EC_{50} value could not be generated; 16% effect at the highest loading level tested, 1021 mg/L.
** 72-hour NOEC

Table 8. Summarized Human Health Data for Members in the Alkyl Acetate C6 to C13 Category

Endpoint	Hexanol, acetate branched and linear alkyl esters (C6-rich)	Acetic acid, C6-8, branched alkyl esters (C7-rich)	Acetic acid, C7-9, branched alkyl esters (C8-rich)	Acetic acid, C8-10, branched alkyl esters (C9-rich)	Acetic acid, C9-11, branched alkyl esters (C10-rich)	Acetic acid, C11-14, branched alkyl esters (C13-rich)
	88230-35-7	90438-79-2	108419-32-5	108419-33-6	108419-34-7	108419-35-8
Acute Oral Toxicity (rat)	>2 g/kg bw	>2 g/kg bw (ra)		>5 g/kg bw	>3 g/kg bw (ra)	>3 g/kg bw
Acute Dermal Toxicity (rabbit)	>3.16 g/kg bw	>3.16 g/kg bw	>3.16 g/kg bw	>3.16 g/kg bw	>3.16 g/kg bw	>3.16 g/kg bw
Irritation	Mild irritant (eyes) Moderate irritant (skin)	Mild irritant (eyes) (ra) Mild to moderate irritant (skin) (ra)				Mild irritant (eyes) Mild irritant (skin)
Mutagenicity Ames Assay	Negative	Negative	Negative	Negative (ra)		Negative
Mutagenicity Mouse Micronucleus	Negative (ra)		Negative	Negative (ra)		Negative
Repeat Dose Toxicity (rat)	NOAEL = 1.0 g/kg/day	NOAEL = 1.0 g/kg/day (ra)	NOAEL = 1.0 g/kg/day	NOAEL = 1.0 g/kg/day (ra)		NOAEL = 1.0 g/kg/day
Reproductive Toxicity (rat)	NOAEL (m,f) = 100 mg/kg/day (ra)		NOAEL (m,f) = 100 mg/kg/day	NOAEL (m,f) = 100 mg/kg/day (ra)		NOAEL (m,f) = 500 mg/kg/day
Developmental Toxicity (rat)	NOAEL (f) = 100 mg/kg/day (ra) NOAEL (p) = 500 mg/kg/day (ra)		NOAEL (f) = 100 mg/kg/day NOAEL (p) = 500 mg/kg/day	NOAEL (f) = 100 to 500 mg/kg/day (ra) NOAEL (p) = 500 to 2500 mg/kg/day (ra)		NOAEL (f) = 500 mg/kg/day NOAEL (p) = 2500 mg/kg/day

bw body weight
(ra) read-across data
(m) male
(f) female
(p) pup

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IUCLID

Data Set

Existing Chemical	:	ID: 88230-35-7
CAS No.	:	88230-35-7
TSCA Name	:	Hexanol, acetate, branched and linear
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Status	:	
Memo	:	ExxonMobil HPV
Printing date	:	19.04.2005
Revision date	:	
Date of last update	:	19.04.2005
Number of pages	:	31
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C6 branched and linear alkyl acetate ester

07.12.2000

Exxate 600

09.02.2001

Oxo-hexyl acetate

27.05.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -59 °C
Sublimation	:	
Method	:	other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: Hexyl acetate ester
Method	:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Remark	:	EPIWIN is used and advocated by the USEPA for chemical property estimation.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (2)

2.2 BOILING POINT

Value	:	= 164 - 176 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078 Mod
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

04.06.2004 (15)

2.3 DENSITY

Type	:	relative density
Value	:	= .87 at 20 °C
Method	:	other: ASTM D891
Year	:	
GLP	:	no data
Test substance	:	other TS

Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint
04.06.2004		(15)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 1.93 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester
Test condition	:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
19.04.2005		(2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 2.83 at 25 °C
pH value	:	
Method	:	other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester
Test condition	:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data

are calculated and not measured.

Flag : Critical study for SIDS endpoint
19.04.2005 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 309 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester
Test condition	:	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	no
Test substance	:	other TS: hexyl acetate ester
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : Hexyl acetate ester
Flag : Critical study for SIDS endpoint
19.04.2005

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000074355 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no data
Test substance : other TS: hexyl acetate ester

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
17.3	7.43 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : Hexyl acetate ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
19.04.2005 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : = 13 day(s) at 25 °C
t1/2 pH 9 : = 36 day(s) at 15 °C
Deg. product : not measured
Method : OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year : 1992
GLP : yes
Test substance : other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Result : Half life at pH 9 and 25 Deg C = 13 days.
Half life at pH 9 and 15 Deg C = 36 days.

The test substance was hydrolytically stable at pH 4, and pH 7 as it degraded less than 5% in 5 days.

Test substance hydrolysis was observed at pH 9 with 35% degradation observed after Day 1 and 95% at Day 5. Test substance measured analytically by GC-FID.

Test condition : The hydrolysis of the test substance was evaluated at 3 relevant pH values. A preliminary test of 95ug/ml at pH values of 4, 7, and 9, showed stability at pH 4 and pH 7. A definitive test was performed at 98ug/ml and a pH value of 9 at varying temperatures (15 and 25 Deg C).
Sufficient volumes of test substance stock solution were added to buffer solution to yield a nominal concentration of 98ug/ml (less than half of expected water sol. conc.). Samples were stored in the dark in laboratory incubators and the temperature recorded daily.

Test vessels were sterilized VOA vials containing buffer solutions of the test substance, with no headspace.

Test substance : CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Conclusion : Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 25 Deg C and the pH is at or below 7.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (6)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	1998
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 144.22 g/mol Water solubility = 309 mg/L Vapour pressure = 193 Pa log Kow = 2.83 Melting point = -59 deg C
Result	:	Air- 91.9% Water- 5.0% Soil- 3.0% Sediment - <0.1% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	Hexyl acetate ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (19)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: Domestic activated sludge, raw sewage, and soil
Contact time	:	28 day(s)
Degradation	:	= 76.9 (±) % after 28 day(s)
Result	:	readily biodegradable
Deg. product	:	

Method	:	EPA OTS 796.3100
Year	:	1988
GLP	:	yes
Test substance	:	other TS: CAS No. 110-82-7; C6 methyl-branched and linear alkyl acetate ester

Result : Half-life was <=2 weeks. By day 28, 76.9% degradation of the test material was observed. 10% biodegradation was achieved on approximately day 2, 50% biodegradation on approximately day 13.
By day 7, >60% biodegradation of positive control was observed. No excursions from the protocol were noted.
Biodegradation was based on theoretical Carbon Dioxide values and the cumulative Carbon Dioxide produced by the test substances.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Substance	74.6, 82.0, 74.1	76.9
Aniline	86.5, 83.7, 83.9	84.7

* replicate data

Test Substance
% Degradation
(mean of replicate data)
Day 2 = 9.7
Day 5 = 30.7
Day 13 = 55.8
Day 19 = 68.2
Day 28 = 76.9

Test condition : Although this test procedure uses an acclimated inoculum, the study was conducted with a non acclimated inoculum that contained activated sludge, raw sewage, and soil. The inoculum and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).
Test vessels were 2L Gledhill flasks located in the dark in an environmental chamber. Each test vessel was monitored for carbon dioxide via charcoal tube and air purging. Sampling was performed on Days 2, 3, 5, 7, 13, 19, and 28.
Test material and positive control were tested in triplicate.
Test material concentration was 30mg carbon/L. Aniline (positive control) concentration was 20 mg carbon/L.
Test temperature was 19 to 23 Deg C.

Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

19.04.2005 (3)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at °C
Concentration	:	
BCF	:	= 30
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no data
Test substance	:	other TS: hexyl acetate ester

Remark	:	A log BCF of 1.5 (BCF = 30) is calculated. Hexyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCCCCCC
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag 19.04.2005	:	Critical study for SIDS endpoint

(1)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LL50	:	= 11.9 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Result	:	96 hour LL50 = 11.9 mg/L (95% CI 10.6 to 13.4) based upon nominal values. The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

Nominal Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
0.5	0
1.3	0
3.2	0
8.0	1
20.0	15

*15 fish added at test initiation
Statistical Method: Trimmed Spearman Karber Method

Test condition	:	The analytical method measured Total Organic Carbon (TOC). TOC was monitored throughout the study in new and old exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TOC for each level tested. No significantly high or low levels were seen. Individual exposure solutions were prepared by adding the test substance to 17L of laboratory blend water in 20L glass carboys. The solutions were mixed for 24 hours at test temp (13-17 Deg C) with a vortex of <10%. Mixing was performed using a magnetic stir plate and teflon stir bar (132 rpm). After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via a glass tube from the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.5L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Three replicates of each concentration were tested, each containing 5 fish. Approximately 80% of each solution was renewed daily from a freshly prepared WAF. Nominal treatment levels were control, 0.5, 1.3, 3.2, 8.0, and 20.0mg/L Test temperature was 15.2 Deg C. Lighting was 62 to 69 ft. candles with gradual 16 hrs light and 8 hrs dark. Dissolved oxygen was 9.0 to 9.4mg/L for "new" solutions and 6.3 to 8.5mg/L for "old" solutions. The pH ranged from 7.4 to 7.7 for "new" solutions and 7.0 to 7.4 for "old" solutions. Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.333g; mean total length=3.6cm; test loading=0.37g of fish/L.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
LL50	:	= 7.6 measured/nominal
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Result : 48 hour LL50 = 7.6 mg/L (95% CI 5.9 to 10.7mg/L) based upon nominal values.

Analytical method used was Total Organic Carbon (TOC).

Nominal Conc. (mg/L)	Daphnia Total Mortality (@48 hrs)*
Control	1
0.1	2
0.5	1
1.0	3
5.0	5
10.0	14

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.
Statistical Method: Finney, D.J. probit procedure of SAS

The analytical method measured Total Organic Carbon (TOC). TOC was monitored throughout the study in new and old exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TOC for each level tested. No significantly high or low levels were seen.

Test condition : Individual exposure solutions were prepared as water accommodated fractions (WAFs). A WAF was prepared by adding test substance to 1.8L of solution in a 2.0 liter aspirator bottle and mixing with a magnetic stir plate and bar. Mixing vortex was <10%. After mixing for 24 hours at room temperature, the WAF was allowed to settle for one hour and removed from the port at the bottom of the bottle.
Test vessels were 125ml glass beakers filled with 140ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 5 organisms.
Nominal treatment levels were: control, 0.1, 0.5, 1.0, 5.0, and 10.0mg/L
Test temperature was 20.7 Deg C. Lighting was 58 to 59 ft candles with 16 hrs light and 8 hrs dark. Dissolved oxygen was 7.3 to 8.8mg/L. The pH ranged from 7.3 to 8.3.

Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 14 to 18 days old.

Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (7)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
EL50 (biomass)	:	= 40.1 measured/nominal
EL50 (growth rate)	:	= 32.1 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Result :

96 hour EL50b = 40.1 mg/L (biomass) based upon nominal values
96 hour EL50gr = 32.1 mg/L (growth rate) based upon nominal values
NOELRb = 31.0 mg/L (biomass) based upon nominal values
NOELRgr = 8.0 mg/L (growth rate) based upon nominal values

No excursions from the protocol were noted.

Nominal Conc. (mg/L)	Mean Growth - 72 & 96 hr (% Inhibition)		Cell Conc. - 96 hr (cells/ml)
Control	n/a	n/a	8.8 x10(5)
8.0	1.2	-4.2*	1.1 x10(6)
31.0	8.4	-3.5*	1.1 x10(6)
62.0	80.2	84.4	2.6 x10(4)
125.0	94.5	97.2	9.6 x10(3)
250.0	99.9	100.0	3.4 x10(3)

n/a - Not applicable
*Stimulatory response
Statistical Method: Proc regression procedure of SAS, Anova procedure of SAS for NOEC

The analytical method measured Dissolved Organic Carbon (DOC). DOC was monitored throughout the study in new and old exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of DOC for each level tested. No significantly high or low levels were seen.

Test condition : Individual exposure solutions were prepared as Water Accommodated Fractions (WAFs). Test material was added to 1.8L of algal media in 2.0L aspirator bottles. The mixing vessels were sealed with foil covered stoppers and mixed on magnetic stir plates with teflon coated stir bars for 24 hours at room temperature. After mixing the solutions were allowed to settle for one hour and the WAF was removed from the bottom of the mixing vessel via the port and used for testing. Test vessels were 125ml glass Erlenmeyer flasks that were completely filled (140ml) with treatment solution and inoculated with algae. Samples were taken daily for cell counts. Four replicates were prepared for each treatment level. The initial algal concentration was 1.0 x 104 cells/ml. All test replicates were placed on a shaker table at 100 oscillations per minute during the study. To facilitate mixing, with no headspace, 10 glass beads were placed in each vessel. Biomass was calculated as the area under the growth curve. Nominal treatment levels were 8.0, 31.0, 62, 125, and 250mg/L

Test temperature was 23.6 Deg. C. Lighting was continuous at 4300 to 4663 Lux. The pH was 7.5 at test initiation and ranged from 8.3 to 10.4 at

test termination.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (5)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 10000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male
Number of animals	:	5
Vehicle	:	other: Corn oil (1.0 % or 10 % v/v)
Doses	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1963
GLP	:	no
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Oral Gavage. Number of animals per dose = 5. Doses: 34.6, 120, 417, 1450, 5000, or 10,000 mg/kg. Single dose following 3-4 hour-fast. Post dose observation period: 1, 4, and 24 hours postdosing and daily for 14 days. One animal at the 1450 mg/kg dose level died on day 11. No toxic signs were observed prior to death and a normal body weight-gain was recorded at death. Postmortem examination showed congestion of the lungs, kidneys, adrenals, and pancreas, and gaseous distention of the stomach and large intestine at the time of death. All other animals showed no gross pathology following termination. Principal toxic effects seen only at the 10,000 mg/kg dose were depression, ataxia, sprawling of limbs and depressed righting reflex only at the 24-hour observation.
Conclusion	:	The acute oral LD50 for C6 branched and linear alkyl acetate ester in male Sprague-Dawley rats is >10 g/kg.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.

19.04.2005 (16)

Type	:	other: Limit
Value	:	> 2000 mg/kg bw
Species	:	rat
Strain	:	other: Crl:CDBR
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: none
Doses	:	2000 mg/kg
Method	:	other: Experimental (EU Annex V, B.1 and OECD 401)
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Oral Gavage. Number of animals per dose per sex = 5. Single Dose of 2000 mg/kg. Post dose observation period 14 days. There was one female death on Day 0 at the 2-hour observation considered to be the result of test material aspiration during dosing.

Clinical signs of toxicity were limited to nasal, oral and/or ocular discharge, abdominal and/or anogenital staining, and/or soft stool in four males at the Day 0 interval. One male and 4 females were free of abnormalities during the entire study. No gross abnormalities were seen at postmortem examination.

Conclusion : C6 branched and linear alkyl acetate ester, did not elicit signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the male animals on Day 0. There was one female death on Day 0, but the death was the result of test material aspiration, not toxicity.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint

19.04.2005 (10)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : other: Limit
Value : > 3160 mg/kg bw
Species : rabbit
Strain : other: albino
Sex : male/female
Number of animals : 1
Vehicle : other: none
Doses :
Method : other: Experimental (Non-regulatory)
Year : 1963
GLP : no
Test substance : other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)

Remark : Dermal Application. Number of animals per dose per sex = 1. Doses: 50, 200, 794 or 3160 mg/kg. Single application / 24-hour occlusive patch. Post dose observation period 14 days.

Two animals, 200 and 3160 mg/kg dosage levels, showed soft feces or diarrhea for two to four days. One animal, 794 mg/kg dosage level, showed diarrhea during the second week and weight loss at termination. All other animals were normal and showed body weight gains. There were no gross pathological findings at the study termination.

Conclusion : C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

19.04.2005 (18)

Type : other: Limit
Value : > 2000 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 5
Vehicle : other: none
Doses : 2000 mg/kg

Method	:	other: Experimental (EU Annex V, B.3; OECD 402)
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Route of administration - Dermal. Number of animals per dose per sex = 5. Single application / 24-hour occlusive patch with 2000 mg/kg. Post dose observation period 14 days. There were no signs of systemic toxicity. Slight dermal irritation was noted in all animals, with the most severe response being observed at the Day 1 observation interval. At post mortem examination, all animals had desquamation at the dose site. In general, dermal responses were considered minimal and transient in nature.
Conclusion	:	C6 branched and linear alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (9)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	100 %
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	other: none
PDII	:	3.08
Result	:	moderately irritating
Classification	:	
Method	:	other: EU Annex V, B.4; OECD 404
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Primary dermal irritation with male New Zealand White rabbits. Number oa animals per dose = 6. Dermal application - single application / 4-hour semi-occlusive patch of 0.5 ml. Post dose observation period 1, 24, 48, and 72 hours and Day 7. Vehicle: none. All animals survived to study termination, were free of clinical signs, and displayed an increase in body weight during the test period. All animals showed erythema and edema in the first 72 hours. The mean scores were 1.72 (erythema) and 1.17 (edema). All animals were free of erythema and edema at the day 7 observation and the study was terminated.
Conclusion	:	C6 branched and linear alkyl acetate ester is a moderate dermal irritant to rabbit skin.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (14)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	100 %
Dose	:	.1 ml
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	
Result	:	slightly irritating
Classification	:	
Method	:	other: Experimental (Non-regulatory)
Year	:	1963
GLP	:	no
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Draize Ocular Irritation with albino rabbits. Single application of neat material of 0.1 ml into the conjunctival sac of the left eye using the untreated right eye as a control. Post dose observation period 1, 4, and 24 hours postdosing and at 2, 3, 4 and 7 days. Vehicle: none. Ocular irritation was most prominent at the 1-hour observation when the total Draize scores ranged from 8 to 12 (Maximum possible score = 110). Irritation was confined to the conjunctivae and generally consisted of moderate redness, chemosis and discharge. The signs of eye irritation completely subsided in all animals by day 7. Fluorescein examination on day 7 confirmed the absence of any corneal damage.
Result	:	Minimal irritation.
Conclusion	:	C6 branched and linear alkyl acetate ester was a mild reversible irritant (Draize Score = 12) causing minimal irritation.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.

19.04.2005 (17)

Species	:	rabbit
Concentration	:	100 %
Dose	:	.1 ml
Exposure time	:	
Comment	:	
Number of animals	:	6
Vehicle	:	none
Result	:	slightly irritating
Classification	:	
Method	:	other: EU Annex V, B.5; OECD 405
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Draize Ocular Irritation with male New Zealand White rabbits. Single instillation of neat material of 0.1 ml into the conjunctival sac of the right eye using the untreated left eye as a control. Post dose observation period 1, 24, and 48 hours postdosing. Vehicle: none. Ocular irritation was most prominent at the 1-hour observation when the total Draize scores ranged from 10 to 12 (Maximum possible score = 110).

Irritation was confined to the conjunctivae and generally consisted of redness, chemosis and discharge. The signs of eye irritation completely subsided in all animals by the 72-hour evaluation. Fluorescein examination at 72 hours confirmed the absence of any corneal damage.

Result	:	Minimal Irritation.
Conclusion	:	C6 branched and linear alkyl acetate ester was a mild reversible irritant (Draize Score = 12).
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (13)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	other: Crl:CD BR
Route of admin.	:	gavage
Exposure period	:	28 day
Frequency of treatm.	:	once/day
Post exposure period	:	
Doses	:	0, 100, 500, and 1000 mg/kg/day
Control group	:	yes
NOAEL	:	= 1000 - mg/kg
Method	:	other: EU Annex V, B.7; OECD 407
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	28-Day repeated dose oral toxicity. Doses: 0, 100, 500, and 1000 mg/kg/day. Volume: 5 ml/kg. Vehicle: Corn oil.
Conclusion	:	Oral administration of C6 branched and linear alkyl acetate ester daily to rats for 28 days did not produce any signs of overt systemic toxicity at any dose level tested. There were no treatment-related clinical in-life, gross postmortem or microscopic findings (including adrenal glands, heart, kidneys, liver, lung, spleen, testes and ovaries); no treatment-related mortality; and no adverse effects on body weight, food consumption, clinical laboratory parameters, or organ weights.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (8)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	other: Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of testing	:	Bacterial
Test concentration	:	250, 500, 1000, 2000, and 3000 µg/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with

Result	:	negative
Method	:	other: EU Annex V, B.14; OECD 471
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	Species/Strain - S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538. Species/cell type - Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9). Vehicle: DMSO. C6 branched and linear alkyl acetate ester, did not induce significant increases in revertant colonies (> 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. Toxicity was observed in both the initial and repeat assays in the following strains and dose levels: TA98 at 2000 µg/plate without metabolic activation, and at 3000 µg/plate with and without metabolic activation; TA100 at 2000 and 3000 µg/plate with and without metabolic activation; TA1535 at 2000 µg/plate without metabolic activation; TA1537 at 250, 500, 1000, 2000, and 3000 µg/plate without metabolic activation; and TA1538 at 1000 and 2000 µg/plate without metabolic activation, and at 3000 µg/plate with and without metabolic activation. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.
Test condition	:	There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 250, 500, 1000, 2000, and 3000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 ºC for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.
Conclusion	:	C6 branched and linear alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested, but was toxic in all strains tested under the conditions of this study.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint
19.04.2005		(12)

Type	:	other: In Vitro Chromosomal Aberration Assay in CHO Cells
System of testing	:	Cultured Chinese hamster ovary (CHO) cells
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	

Method	:	other: Galloway, et al, Development of a standard protocol for in vitro cytogenetic testing with Chinese hamster ovary cells: comparison of results for 22 compounds in two laboratories. Environ. Mutagen. 7:1-51, 1985.
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 88230-35-7; Hexanol, acetate, branched and linear ester, C6 (>95%)
Remark	:	C6 branched and linear alkyl acetate ester, reduced cell survival by at least 50% when compared to the vehicle control in the repeat assay: 20-hour harvest without activation and 44-hour harvest with and without metabolic activation. All negative and positive controls used in this study performed in an appropriate manner.
Result	:	C6 branched and linear alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was no evidence of a positive dose response nor of any treated group being different from the control in these analyses. For the repeat harvest, the high dose group (550 mg/mL) was statistically different from the vehicle control ($p<0.05$). However, this statistically significant finding (6.5% aberrant cells) was not reproducible. No increase was observed at the 44-hour harvest time. In addition, no increase was observed in the initial assay with metabolic activation at similar dose levels. There was no statistically significant finding in the 44-hour harvest.
Test condition	:	Treatment group doses (14 total in initial and repeat assays) ranged from 250-480 mg/mL in the 20-hour initial test; 230-550 mg/mL in the 20- and 44-hour repeat assays. S9 activation was used in doses ranging from 350-480 mg/mL in the 20-hour initial assay and ranging from 380-550 mg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1.0% final volume to ensure normal cell viability and growth rate). Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.
Conclusion	:	C6 branched and linear alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 550 mg/mL with and 430 mg/mL without metabolic activation.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag 19.04.2005	:	Critical study for SIDS endpoint

(11)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(2) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(3) Exxon Biomedical Sciences Inc. 1994. Aerobic Aquatic Biodegradation, Gledhill Shake Flask Test. Study #168687.

(4) Exxon Biomedical Sciences Inc. 1995. Acute Fish Toxicity Test with Rainbow Trout. Study #101558.

(5) Exxon Biomedical Sciences Inc. 1995. Algal Inhibition Test. Study #101567.

(6) Exxon Biomedical Sciences Inc. 1995 Abiotic Degradation Hydrolysis as a Function of pH. Study #101590.

(7) Exxon Biomedical Sciences, Inc. 1995. Acute Daphnid Toxicity Test. Study #101542B.

(8) Exxon Biomedical Sciences, Inc., East Millstone, NJ, 28-Day Repeated Dose Oral Toxicity Study in the Rat; Project # 101570.

(9) Exxon Biomedical Sciences, Inc., East Millstone, NJ, Acute Dermal Toxicity Study in the Rabbit; Project # 101506.

(10) Exxon Biomedical Sciences, Inc., East Millstone, NJ, Acute Oral Toxicity Test in the Rat; Project # 101501.

(11) Exxon Biomedical Sciences, Inc., East Millstone, NJ, In Vitro Chromosomal Aberration Assay in CHO Cells, Project # 101532.

(12) Exxon Biomedical Sciences, Inc., East Millstone, NJ, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Assay; Study # 101525.

(13) Exxon Biomedical Sciences, Inc., East Millstone, NJ, Ocular Irritation Study in Rabbit without Eyewash; Project # 101513.

(14) Exxon Biomedical Sciences, Inc., East Millstone, NJ, Primary Dermal Irritation Study in the Rabbit; Project # 101504.

(15) ExxonMobil Chemical Company (2003). Exxate 600 Data Sheet.

(16) Hazleton Laboratories Incorporated, Falls Church, VA, Project # 38355.

(17) Hazleton Laboratories Incorporated, Falls Church, VA; Project # 38355.

(18) Hazleton Laboratories, Inc., Falls Church, VA; Project # 38355.

(19) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

Memo : EU RIsk assessent final draft

08.06.2001

IUCLID

Data Set

Existing Chemical	:	ID: 90438-79-2
CAS No.	:	90438-79-2
TSCA Name	:	Acetic acid, C6-8-branched alkyl esters
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Status	:	
Memo	:	ExxonMobil HPV
Printing date	:	19.04.2005
Revision date	:	
Date of last update	:	19.04.2005
Number of pages	:	33
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C6 - C8 branched alkyl acetate ester

27.02.2004

Exxate 700

27.02.2004

oxo-heptyl acetate

04.06.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -50 °C
Sublimation	:	
Method	:	other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no data
Test substance	:	other TS: C7 methyl-branched alkyl acetate ester
Method	:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Remark	:	EPIWIN is used and advocated by the USEPA for chemical property estimation.
Test substance	:	C7 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (3)

2.2 BOILING POINT

Value	:	= 176 - 200 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078 Mod
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

04.06.2004 (15)

2.3 DENSITY

Type	:	relative density
Value	:	= .87 at 20 °C
Method	:	other: ASTM D891
Year	:	
GLP	:	no data

Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (15)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 1.035 hPa at 25 °C
Decomposition	:	
Method	:	OECD Guide-line 104 "Vapour Pressure Curve"
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	Sorbent trap extraction samples were analyzed using gas chromatography. Average Vapor Pressure per temperature: 24 Deg C (room temp) 96.38 Pa 35 Deg C 214.3 Pa 45 Deg C 438.8 Pa 25 Deg C 103.5 Pa (estimated from linear regression)
Test condition	:	The test substance was coated onto glass beads, which were then transferred to saturator columns. Three columns were prepared for each temperature evaluation (9 total). The Vapor Pressure was evaluated at temperatures of 24, 35, and 45 Deg C. A stream of inert carrier gas (N2) was passed over the separator columns and became saturated with the test substance vapors. The test substance vapors were then adsorbed to charcoal sorbent tubes. Sorbent tubes were extracted with 2% acetone in carbon disulfide. Vapor pressure determination interval was 2 hours at 24 Deg C and 1 hour at 35 and 45 Deg C. The N2 flow rate was 50ml/min at each temperature evaluation.
Test substance	:	CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (8)

Value	:	= .68 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS
Test condition	:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods

use boiling point for the calculation.

The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990.

A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.

Test substance : CAS No. 90438-79-2; Acetic acid, C6-8 branched and linear
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
04.06.2004 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : 3.9 - 4.2 at °C
pH value :
Method : OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year : 1989
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : The test substance eluted as several groups. One group was estimated to have a Log Pow of < 0.3. The second group had a Log Pow values ranging from 1.7 to 4.4. The three major components C6, C7, C8 acetates had Log Pow values of 3.9, 4.0, and 4.2 respectively.

The retention time for the 3 major components were 7.66, 8.04, and 8.71 minutes.

All values were measured using High Performance Liquid Chromatography (HPLC).

Test condition : The test substance was evaluated as a 5.3% solution in HPLC grade methanol. Six reference compounds were also evaluated in a combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) of 75% methanol and 25% distilled water. The pH of both solutions was 6.5.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (6)

Partition coefficient : octanol-water
Log pow : = 3.32 at 25 °C
pH value :
Method : other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year :
GLP : no data
Test substance : other TS

Test condition : Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-

92.

Test substance	:	CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.06.2004 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 158 mg/l at 20 °C
pH value	:	3.5 - 4.9
concentration	:	at 20 °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	OECD Guide-line 105
Year	:	1995
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	Water solubility = 158 mg/L. Samples measured over three equilibration days on three separate replicates. Day 1 154 mg/L pH 3.5 Day 2 154 mg/L pH 4.9 Day 3 162 mg/L pH 4.3 The clear aqueous solution was analytically measured by gas chromatography using mass selective detection (GC-MSD).
Test condition	:	A total of 9 test systems were prepared. Three replicates for each of three equilibration days. The test systems consisted of glass distilled water and a loading of ~600mg/L of test substance. The test vessels were 25ml screw cap centrifuge tubes containing ~30ml of solution (no headspace). The test systems were agitated on an incubator shaker for the designated number of days at 30 Deg C, between 25 and 50 rpm. Samples were then transferred to a 20 Deg C incubator and agitated an additional 24 hours. The solutions were then centrifuged at 5000 rpm for 15 minutes and returned to the 20 Deg C incubator for another hour to ensure correct temperature at sampling. The surface test material and the next 10-15 ml were removed. The analytical samples were removed from the remaining (bottom) solution into a headspace sample vial.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (7)

Solubility in	:	Water
Value	:	= 102 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	

Deg. product	:	
Method	:	other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year	:	
GLP	:	no data
Test substance	:	other TS
Test condition	:	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

04.06.2004 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	no
Test substance	:	other TS: C7 methyl-branched alkyl acetate ester
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : CAS No. 90438-79-2; Acetic acid, C6-8 branched and linear
Flag : Critical study for SIDS endpoint
19.04.2005

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000088486 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance : other TS: C7 methyl-branched alkyl acetate ester

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
14.5	8.85 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : C7 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
19.04.2005

(3)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at 50 °C
t1/2 pH7 : = 24.3 day(s) at 50 °C
t1/2 pH9 : = 5.3 day(s) at 30 °C
t1/2 pH 9 : = 15.6 - 16 day(s) at 20 °C
Deg. product : not measured
Method : OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year : 1997
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : Hydrolysis at pH 4 is stable (<10% degradation over 5 days).

Test substance hydrolysis was observed at pH 9 and a slower but measurable hydrolysis occured at pH 7.

Test condition : The hydrolysis of the test substance was evaluated at 3 relavent pH values. A preliminary test at pH values of 4, 7 and 9, showed stability at pH 4. A definitive test was performed at pH values of 7 and 9 at varying temperatures (20 and 30 Deg C for pH 9; 40 and 50 Deg C for pH 7). Sufficient volumes of test substances stock solution were added to buffer solution to yield nominal concentration less than 60ug/L (40-53 ug/L) (half of expected water sol. conc.). Samples were stored in the dark in laboratory incubators and the temperature recorded daily.

Test vessels were sterilized VOA vials containing buffer solutions of the test substance, with no headspace.

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Conclusion : Hydrolysis of the test substance is not expected to be a significant mechanism of abiotic degradation in natural bodies of water where the temperature is generally less than 20 Deg C and the pH is at or below 7.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005

(9)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	1998
Method	:	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). Input values used: Molecular mass = 158.24 g/mol Water solubility = 102 mg/L Vapour pressure = 68 Pa log Kow = 3.32 Melting point = -50 deg C
Result	:	Air- 88.0% Water- 4.1% Soil- 7.7% Sediment - 0.2% Suspended Sed - <0.01% Biota - <0.01%
Test substance	:	C7 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (17)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	
Inoculum	:	activated sludge, domestic
Contact time	:	28 day(s)
Degradation	:	(±) % after
Result	:	
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1993

GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	Test material was readily biodegradable. Half-life was <1 week. By day 28, 77% degradation of the test material was observed. 10% biodegradation was achieved on day 1, 50% biodegradation on approximately day 5. By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	73.5, 80.4, 77.4	77.1
Na Benzoate	76.0, 78.3	77.1

* replicate data

Source	:	ExxonMobil Chemicals
Test condition	:	Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride). Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material concentration was 52mg/L. Sodium benzoate (positive control) concentration was 52mg/L. Test temperature was 22 +/- 1 Deg C. All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (5)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at °C
Concentration	:	
BCF	:	= 63
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no data
Test substance	:	other TS: C7 methyl-branched alkyl acetate ester
Remark	:	A log BCF of 1.8 (BCF = 63) is calculated. C7 methyl-branched alkyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCCCC(C)CC
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are

calculated and not measured.

Flag : Critical study for SIDS endpoint
19.04.2005 (2)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 8.18 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2, C6 - C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : 96 hour LC50 = 8.18mg/L (95% CI 5.85 to 11.4) based upon measured values.

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).
The fish were slightly smaller than the guideline suggestion of 4.0 to 6.0cm, which were purposely selected to help maintain oxygen levels in the closed system.

Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	0
1.2	0
1.49	0
5.39	2
21.1	10
43.6	10

*10 fish added at test initiation
Statistical Method: Trimmed Spearman Karber Method

Test condition : Individual test concentrations were prepared by adding the test substance, weighed on teflon disks, to 12 L of laboratory blend water in 13L glass aspirator bottles. The solutions were mixed for 24 hours at room temp (20-24 Deg C) with a vortex of <10% (3 cm vortex). Mixing was performed using a magnetic stir plate and teflon stir bar. After mixing, the solutions were allowed to settle for one hour and the Water Accommodated Fraction (WAF) was removed via port at the bottom of vessel. Test vessels were 4.0L aspirator bottles containing 4.0L of solution (no headspace). Test vessels were sealed with foil covered stoppers. Two replicates of each concentration were tested, each containing 5 fish. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.
Nominal treatment levels were control, 2.0, 4.5, 10.0, 23.0, and 50.0mg/L, which measured: 1.2, 1.49, 5.39, 21.1, and 43.6mg/L, respectively, and are based on the mean of samples taken from the new and old solutions.
Test temperature was 13.6 Deg C. Lighting was 16 hrs light and 8 hrs dark. Dissolved oxygen was 8.3 to 10.4mg/L for "new" solutions and 4.5 to 7.9mg/L for "old" solutions. The pH ranged from 7.3 to 8.4 for "new" solutions and 6.7 to 7.6 for "old" solutions.
Fish supplied by Thomas Fish Co.; age = approximately 6 weeks; mean wt.=0.319g; mean total length=3.5cm; test loading=0.399g of fish/L.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005

(4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	other: Activated sludge - Respiration Inhibition
Species	:	activated sludge of a predominantly domestic sewage
Exposure period	:	30 minute(s)
Unit	:	mg/l
Analytical monitoring	:	yes
Method	:	OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year	:	1997
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	No appreciable inhibition of respiration was measured. The controls were within 11.24% of their mean oxygen consumption rate and the EC50 for the reference substance was 20.8mg/L. Both values fall within the acceptable ranges for study validity (Controls within 15%, and positive substance between 5-30mg/L)
Test condition	:	The test solution consisted of synthetic sewage, activated sludge and reverse osmosis water. To this mixture, the appropriate amount of reference stock or test substance was added (except controls). The test treatments were aerated throughout the 30-minute exposure. After the 30 minute contact time, the contents were poured into a BOD bottle and the Dissolved Oxygen (DO) concentration was measured for 10 minutes or until a DO level of 2.5mg/L was achieved. The respiration rate was determined by the linear slope of DO level vs time. The positive control (3,5-DCP) was tested at concentrations of 5, 15 and 30 mg/L. The test substance was evaluated at concentrations of 5, 10, 25, and 50 mg/L.
Test substance	:	CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Conclusion	:	The test substance did not inhibit the respiration of the sludge medium.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (10)

Type	:	soil
Species	:	aerobic microorganisms
Exposure period	:	28 day(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 216
Year	:	2001
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	Following an initial rise in ammonium concentrations in the soil of all groups, nitrogen transformation was evident from the subsequent decline in ammonium concentrations and gradual increase in nitrate concentrations over the study period.

Statistical evaluation of the ammonium and nitrate data found a number of statistically significant differences in treated soil groups when compared with the non-treated control soil. However, at the end of the 28 day study period, the deviation in measured activity in soils treated with the test substance at 1x PEC (Group 2) and 5x PEC (Group 3) compared to non-treated control soil (Group 1) was less than 25% for both ammonium (0% for Group 2 and Group 3) and for nitrate
(-1.12% and -6.41% for Group 2 and Group 3 respectively).

At the end of the 28 day study period, test soil "treated" with acetone as a solvent control showed values that were comparable (less than 25% different) to the non-treated control soil (Group 1) indicating that the use of acetone as a solvent had not adversely affected the test soil in this study.

Test condition : The test substance (TS) was tested at two treatment concentrations, the lower treatment concentration was equal to the maximum Predicted Environmental Concentration (PEC = 600 ml TS/hectare) and the higher treatment concentration was equal to 5x PEC (3 litres TS/hectare). The test soil was a sandy loam soil obtained from a site at Manningtree, Essex, England which had received no pesticides or fertilisers for at least 3 years prior to sampling.

To determine nitrogen transformation, non-treated control soil (Group 1) and soils treated with the test substance (Group 2 = 1x PEC, Group 3 = 5x PEC), were incubated in the dark at 20 ± 2°C as bulk samples. Each soil group was amended with lucerne meal, as a nitrogen source, at the time of preparation:

Group 1 - 2kg soil + lucerne meal + water
Group 2 - 2kg soil + lucerne meal + water containing 1x PEC
Group 3 - 2kg soil + lucerne meal + water containing 5x PEC

To achieve satisfactory incorporation of the test substance into the test soil, the test substance was first mixed with acetone and then transferred into the distilled water addition (60.7 g distilled water) required to amend the moisture content of the test soil to 40% of its maximum water holding capacity and this water was then sprinkled onto the soil and mixed in thoroughly.

Triplicate portions of each soil group were sampled within 6 hours (Day 0), 7, 14 and 28 days after preparation and then extracted for analysis of ammonium, nitrite and nitrate concentrations using a continuous flow colorimetric autoanalyser.

Analysis of soil

Sand (63 mm - 2 mm): 74.13%
Silt (2 mm - 63 mm): 20.36%
Clay (<2 mm): 5.51%
pH: 6.4
Organic carbon: 0.6%
Maximum water holding capacity: 26.1%
Cation exchange capacity (mEq/100 g): 7.4

Analysis of soil microbial biomass:

Total biomass (BC) mg C/kg soil: 115.17
Microbial biomass: 1.92%
(Total soil organic carbon = 0.6 %)

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Conclusion	:	Based on the results of this study, under anticipated conditions of field use equivalent to both 1x the PEC and 5x the PEC, the test substance did not exhibit a long-term influence on nitrogen transformation activity in soil.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint
19.04.2005		(16)
Type	:	soil
Species	:	aerobic microorganisms
Exposure period	:	28 day(s)
Unit	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 217
Year	:	2001
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	Statistical evaluation of the carbon transformation data found no statistically significant differences between the test soil treated with the test substance at 1x PEC when compared with the non-treated control soil. Statistical evaluation showed statistically significant increased levels of carbon transformation for the 5x PEC treated soil when compared with the non-treated control soil on Days 7, 14 and 28. At the end of the 28 day study period, the deviations in carbon transformation in soils treated with the test substance at 1x PEC (Group 2) compared to non-treated control soil (Group 1) were less than 25%, ranging from -5.5% to +3.4%. However carbon transformation in soil treated with the test substance at 5x PEC (Group 3) was substantially increased on Day 28 compared to non-treated control soil (Group 1), ranging from +27.0% to +109.2%. At the end of the 28 day study period, test soil "treated" with acetone as a solvent control showed values that were comparable (less than 25% different) to the non-treated control soil (Group 1) indicating that the use of acetone as a solvent had not adversely affected the test soil in this study.
Test condition	:	The test substance (TS) was tested at two treatment concentrations, the lower treatment concentration was equal to the maximum Predicted Environmental Concentration (PEC = 600 ml TS/hectare) and the higher treatment concentration was equal to 5x PEC (3 litres TS/hectare). The test soil was a sandy loam soil obtained from a site at Manningtree, Essex, England which had received no pesticides or fertilisers for at least 3 years prior to sampling. To determine carbon transformation, non-treated control soil (Group 1) and soils treated with the test substance (Group 2 = 1x PEC, Group 3 = 5x PEC), were incubated in the dark at 20 ± 2°C as bulk samples: Group 1 - 2kg soil + lucerne meal + water Group 2 - 2kg soil + lucerne meal + water containing 1x PEC Group 3 - 2kg soil + lucerne meal + water containing 5x PEC To achieve satisfactory incorporation of the test substance into the test soil, the test substance was first mixed with acetone and then transferred into the distilled water addition (60.7 g distilled water) required to amend the moisture content of the test soil to 40% of its maximum water holding capacity and this water was then sprinkled onto the soil and mixed in thoroughly. Triplicate portions of each soil group were sampled on Day 0, 7, 14 and 28 and treated with glucose to elicit an immediate glucose induced maximum

respiratory response. Respiration rates were determined at regular intervals over 12 consecutive hours using an ADC 2250 Infrared Gas Analyser.

Analysis of soil

Sand (63 mm - 2 mm): 74.13%
Silt (2 mm - 63 mm): 20.36%
Clay (<2 mm): 5.51%
pH: 6.4
Organic carbon: 0.6%
Maximum water holding capacity: 26.1%
Cation exchange capacity (mEq/100 g): 7.4

Analysis of soil microbial biomass:

Total biomass (BC) mg C/kg soil: 115.17
Microbial biomass: 1.92%
(Total soil organic carbon = 0.6 %)

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Conclusion : Based on the results of this study, under anticipated conditions of field use equivalent to 1x PEC, the test substance did not exhibit a long-term influence on carbon transformation activity in soil. When applied at a rate equivalent to 5x PEC, the test substance did show a stimulation of carbon transformation activity by soil microorganisms. This increase in carbon transformation activity as measured by an increase in carbon dioxide evolution is believed to have resulted from the mineralization of test substance by the soil microbial population.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

19.04.2005 (16)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species : other terrestrial plant: Glycine max (soybean)
Endpoint : other: emergence / growth
Exposure period : 17 day(s)
Unit : mg/kg soil dw
LL50 : > 1562 measured/nominal
EL50 : > 1562 measured/nominal
Method : OECD Guide-line 208 "Terrestrial Plants, Growth Test"
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Method : The statistical method used to calculate the LL50 values was a maximum

likelihood analysis based on Finney, D.J., 1971. Probit Analysis, 3rd Edition, London: Cambridge University Press. The EL50 values were determined using the linear interpolation method (Norberg-King, T.J., A Linear Interpolation Method for Sublethal Toxicity: The Inhibition Concentration (ICp) Approach (Version 2.0). July 1993. U.S. Environmental Protection Agency, Environmental Research Laboratory, Duluth MN).

Result : The LL50 (Lethal Loading 50) for Soybean (Glycine max) > 1562 mg/Kg.
The EL50 (Effect Loading 50) for Soybean (Glycine max) > 1562 mg/Kg.

The soybean did not exhibit a lethal effect by test termination at the highest loading tested (1562 mg/Kg). The test substance did exhibit an effect on growth compared to the control (30 percent reduction), but not sufficient to cause a 50 percent effect.

The LL50 (Lethal Loading 50) is the test substance loading level, which exhibits 50% emergence of the test species as compared to the control for a specific exposure period. The EL50 (Effect Loading 50) is the test substance loading level, which exhibits 50% growth of the test species based on weight as compared to the control for a specific exposure period.

Test condition : The test substance soil loading levels for this study were 1562 mg/Kg, 665mg/Kg, 245mg/Kg, and 97mg/Kg. The control treatment consisted of soil with no test substance. The soil used was artificial, composed of a mixture of 89% sand (>/= 50% of the particles between 50 and 200 mm), 1% peat moss (0.5cm sieved to remove coarse fragments) and 10% kaolin clay (96 - 97% kaolinite). The carbon content was 0.37% (2% organic matter). This analysis was not performed in a GLP compliant manner, it is not believed to have affected the results. Fine particles <20 um made up between 13% of the soil (checked by sieving). The artificial soil was not sterilized.

Soil in each loading level and the control was hydrated to 85% of the water holding capacity.

Four replicates were established for each test substance treatment level and control using ten seeds per replicate. Replicate test chambers contained approximately 246g of hydrated soil. Test chambers were glass crystallizing dishes (125 mm X 65 mm).

Mean test temperature: 24.3°C, sd 0.1
Lighting: 16 hour light,8 hour dark photoperiod. Intensity: 3983 - 4349 Lux
Soil pH: 6.9
Soil depth: 2cm

Organism supplier was Carolina Biological Supply Co., Burlington, NC 27215-3398.

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (14)

Species : Raphanus sativus (Dicotyledon)
Endpoint : other: emergence / growth
Exposure period : 17 day(s)
Unit : mg/kg soil dw
LL50 : = 1015 measured/nominal
EL50 : = 446 measured/nominal
Method : OECD Guide-line 208 "Terrestrial Plants, Growth Test"
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Method : The statistical method used to calculate the LL50 values was a maximum likelihood analysis based on Finney, D.J., 1971. Probit Analysis, 3rd Edition, London: Cambridge University Press. The EL50 values were determined using the linear interpolation method (Norberg-King, T.J., A Linear Interpolation Method for Sublethal Toxicity: The Inhibition Concentration (ICp) Approach (Version 2.0). July 1993. U.S. Environmental Protection Agency, Environmental Research Laboratory, Duluth MN).

Result : The LL50 (Lethal Loading 50) for Radish (Raphanus sativus) = 1015 mg/Kg. The EL50 (Effect Loading 50) for Radish (Raphanus sativus) = 446 mg/Kg.

The LL50 (Lethal Loading 50) is the test substance loading level, which exhibits 50% emergence of the test species as compared to the control for a specific exposure period. The EL50 (Effect Loading 50) is the test substance loading level, which exhibits 50% growth of the test species based on weight as compared to the control for a specific exposure period.

Test condition : The test substance soil loading levels for this study were 1562 mg/Kg, 665mg/Kg, 245mg/Kg, and 97mg/Kg. The control treatment consisted of soil with no test substance. The soil used was artificial, composed of a mixture of 89% sand (>/= 50% of the particles between 50 and 200 mm), 1% peat moss (0.5cm sieved to remove coarse fragments) and 10% kaolin clay (96 - 97% kaolinite). The carbon content was 0.37% (2% organic matter). This analysis was not performed in a GLP compliant manner, it is not believed to have affected the results. Fine particles <20 um made up between 13% of the soil (checked by sieving). The artificial soil was not sterilized.

Soil in each loading level and the control was hydrated to 85% of the water holding capacity.

Four replicates were established for each test substance treatment level and control using ten seeds per replicate. Replicate test chambers contained approximately 246g of hydrated soil. Test chambers were glass crystallizing dishes (125 mm X 65 mm).

Mean test temperature: 24.3°C, sd 0.1
Lighting: 16 hour light,8 hour dark photoperiod. Intensity: 3983 - 4349 Lux
Soil pH: 6.9
Soil depth: 2cm

Organism supplier was Carolina Biological Supply Co., Bur

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005 (14)

Species : Avena sativa (Monocotyledon)
Endpoint : other: emergence / growth
Exposure period : 19 day(s)
Unit : mg/kg soil dw
LL50 : = 530 measured/nominal
EL50 : = 225 measured/nominal
Method : OECD Guide-line 208 "Terrestrial Plants, Growth Test"
Year : 2001
GLP : yes
Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Method : The statistical method used to calculate the LL50 values was a maximum likelihood analysis based on Finney, D.J., 1971. Probit Analysis, 3rd

Edition, London: Cambridge University Press. The EL50 values were determined using the linear interpolation method (Norberg-King, T.J., A Linear Interpolation Method for Sublethal Toxicity: The Inhibition Concentration (ICp) Approach (Version 2.0). July 1993. U.S. Environmental Protection Agency, Environmental Research Laboratory, Duluth MN).

Result : The LL50 (Lethal Loading 50) for Oat (Avena sativa) = 530 mg/Kg. The EL50 (Effect Loading 50) for Oat (Avena sativa) = 225 mg/Kg.

The LL50 (Lethal Loading 50) is the test substance loading level, which exhibits 50% emergence of the test species as compared to the control for a specific exposure period. The EL50 (Effect Loading 50) is the test substance loading level, which exhibits 50% growth of the test species based on weight as compared to the control for a specific exposure period.

Test condition : The test substance soil loading levels for this study were 1562 mg/Kg, 665mg/Kg, 245mg/Kg, and 97mg/Kg. The control treatment consisted of soil with no test substance. The soil used was artificial, composed of a mixture of 89% sand (>/= 50% of the particles between 50 and 200 mm), 1% peat moss (0.5cm sieved to remove coarse fragments) and 10% kaolin clay (96 - 97% kaolinite). The carbon content was 0.37% (2% organic matter). This analysis was not performed in a GLP compliant manner, it is not believed to have affected the results. Fine particles <20 um made up between 13% of the soil (checked by sieving). The artificial soil was not sterilized.

Soil in each loading level and the control was hydrated to 85% of the water holding capacity.

Four replicates were established for each test substance treatment level and control using ten seeds per replicate. Replicate test chambers contained approximately 246g of hydrated soil. Test chambers were glass crystallizing dishes (125 mm X 65 mm).

Mean test temperature: 24.3°C, sd 0.1
Lighting: 16 hour light,8 hour dark photoperiod. Intensity: 3983 - 4349 Lux
Soil pH: 6.9
Soil depth: 2cm

Organism supplier was Carolina Biological Supply Co., Burlington, NC

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

19.04.2005

(14)

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

Type	:	artificial soil
Species	:	other: Eisenia foetida
Endpoint	:	mortality
Exposure period	:	14 day(s)
Unit	:	mg/kg soil dw
LL50	:	= 539 measured/nominal
Method	:	OECD Guide-line 207 "Earthworm, Acute Toxcity Test"
Year	:	2001
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Method : The statistical method used to calculate the 7 and 14 day LL50 values for the substance was a maximum likelihood analysis based on Finney, D.J.,

1971. Probit Analysis, 3rd Edition, London: Cambridge University Press.

Result : The 7 day LL50 (Lethal Loading 50) was 639mg/Kg with a 95% confidence interval of 560 - 742mg/Kg. The 14 day LL50 was 539mg/Kg with a 95% confidence interval of 451 - 664mg/Kg. These endpoints are based on the mg of test substance per Kg of soil, dry weight.

Test condition : The test substance soil loading levels for this study were; 871 mg/kg, 409mg/kg, 203mg/kg, 108mg/kg, and 48mg/kg. The control treatment consisted of soil with no test substance. The soil used was artificial and composed of a mixture of 50% sand (³ 50% of the particles between 50 and 200 mm), 20% kaolin clay (96 - 97% kaolinite) and 30% peat moss (no visible plant material, finely ground).

Soil in each loading level and the control was hydrated to an overall moisture content of approximately 55% of the dry weight of the artificial soil.

Four replicates at each loading level were prepared containing 10 worms.

Test chambers were one quart (approximately 950mL) size glass jars. Jars were approximately 17cm high and approximately 9.5cm in diameter, covered with perforated plastic film to minimize volatility and soil moisture loss.

Mean test temperature: 18.7°C, sd 0.2
Continuous lighting: 612 - 660 Lux
Soil pH: 6.7
Soil depth: 16cm

Organism supplier was Carolina Biological Supply Co., Burlington, NC 27215-3398.

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

19.04.2005 (13)

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	other: Limit test
Value	:	> 3160 - mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	3
Vehicle	:	other: none
Doses	:	3160 mg/kg
Method	:	other: Experimental (Non-regulatory)
Year	:	1983
GLP	:	no
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	There were no overt signs of systemic toxicity. Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14. Erythema was noted in all animals at 24 hours, ranging from moderate to severe, and regressed in all animals throughout the study. On Day 14, five of six animals showed very slight erythema and one had no signs of erythema. Edema was evident in all but one animal at 24 hours and by Day 14 all but one animal was free of signs of edema. Desquamation was evident in five animals on Day 14. All animals survived to termination of the study and increased in body weight. There were no significant findings at the postmortem gross examination.
Test condition	:	Single application / 24-Hour Occlusive Patch
Test substance	:	CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Conclusion	:	C6-C8 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	other: Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)
System of testing	:	Bacterial
Test concentration	:	50, 100, 200, 400, 600, and 800 µg/plate (50 during repeat assay only; 800 during initial assay only)
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: EU Annex V, B.14; OECD 471
Year	:	1997
GLP	:	yes
Test substance	:	other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Result	:	C6-C8 branched alkyl acetate ester, did not induce significant increases in revertant colonies (> 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains. Toxicity was observed in the initial assay in the following dose levels and strains: at 100 µg/plate TA1537 (+S9), > 200 µg/plate in TA100 (-S9), TA1535 (+S9), TA1537 (-S9), TA1538 (±S9); > 400 µg/plate in TA98 (±S9), TA1535 (-S9), TA1537 (+S9), and > 600 µg/plate in TA100 (+S9). In the repeat assay, toxicity was observed at doses > 400 µg/plate in TA100 (-S9) and TA1537 (-S9), and at 600 µg/plate in TA98 (-S9), TA1535 (-S9), TA1537 (+S9), and TA1538 (±S9). The nontreated and vehicle controls responded in a manner consistent with data from previous assays.
Test condition	:	Species/Strain : S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538 Species/cell type: Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9) Vehicle: DMSO There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 100, 200, 400, 600, and 800 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top

agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37± 2 ºC for approximately 2 days.

Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

Test substance : CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Conclusion : C6-C8 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested, even at doses that produced evidence of toxicity.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

19.04.2005 (12)

Type : other: In Vitro Chromosomal Aberration Assay in CHO Cells

System of testing : Cultured Chinese hamster ovary (CHO) cells

Test concentration : 80-240 mg/mL in the 20-hour initial test; 40-200 mg/mL in the 20- and 44-hour repeat assays

Cycotoxic concentr. :

Metabolic activation : with and without

Result :

Method : other: Galloway, et al, Development of a standard protocol for in vitro cytogenetic testing with Chinese hamster ovary cells: comparison of results for 22 compounds in two laboratories. Environ. Mutagen. 7:1-51, 1985.

Year : 1997

GLP : yes

Test substance : other TS: CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)

Result : C6-C8 branched alkyl acetate ester, was tested in a 20-hour chromosome aberration assay using Chinese hamster ovary cells with and without metabolic activation. A repeat assay was also performed using 20-hour and 44-hour harvests. For the initial 20-hour harvest data, there was a notable decrease in the percent cell confluency at concentrations >/= 180 mg/mL with activation and at concentrations >/= 140 mg/mL without activation. Cell morphology and mitotic indices were acceptable at or below these levels and cell death was prevalent above these levels. For the repeat assay, there were no statistically significant dose-related trends in the percentage of aberrant cells and none of the test concentrations were statistically different than the vehicle control in the 20 or 44 hour activated or nonactivated series. The percentage of aberrant cells in the vehicle control groups ranged from 1% to 2.0%, and the percentage of aberrant cells in the treated groups ranged from 0.0% to 2.6% for the 20 and 44 hour activated and nonactivated series.

All negative and positive controls used in this study performed in an appropriate manner.

Test condition : Treatment group doses (11 total in initial and repeat assays) ranged from 80-240 mg/mL in the 20-hour initial test; 40-200 mg/mL in the 20- and 44-hour repeat assays. S9 activation was used in doses ranging from 80-240 mg/mL in the 20-hour initial assay and ranging from 40-200 mg/mL in the 20- and 44-hour repeat assays. Vehicle in all assays was DMSO (not exceeding 1.0% final volume to ensure normal cell viability and growth rate).

Positive controls, N-methyl-N-Nitro-N-Nitrosoguanidine (MNNG - clastogen that does not require metabolic activation) and 7,12-Dimethylbenz[a]anthracene (DMBA- clastogen that requires metabolic activation) were used as positive controls in the nonactivated series and activated series, respectively.

Test substance	:	CAS No. 90438-79-2; C6-C8 methyl-branched alkyl acetate ester, predominantly C7 (>85%)
Conclusion	:	C6-C8 branched alkyl acetate ester was considered negative for inducing chromosome aberrations under the conditions of this test at doses up to 180 mg/mL with and 140 mg/mL without metabolic activation.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (11)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bio/dynamics Inc. 1983. Acute Dermal Toxicity Study in the Rabbit with C6-C8 Branched Alkyl Acetate Ester. Project # 321106.

(2) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(3) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(4) Exxon Biomedical Sciences Inc. 1997. Acute Fish Toxicity Test with Rainbow Trout. Study #164058.

(5) Exxon Biomedical Sciences Inc. 1998 Ready Biodegradability, Manometric Respirometry. Study #164094A.

(6) Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #164087D.

(7) Exxon Biomedical Sciences Inc. 1998. Water Solubility Test (Flask Method). Study #164038.

(8) Exxon Biomedical Sciences Inc. 1998. Vapor Pressure (Gas Saturation Method). Study #164086D.

(9) ExxonBiomedical Sciences Inc. 1997, Hydrolysis as a function of pH 164090H.

(10) ExxonMobil Biomedical Sciences Inc. 1997. Activated Sludge Respiration Inhibition Test. Study #164094B.

(11) ExxonMobil Biomedical Sciences, Inc. 1997. In Vitro Chromosomal Aberration Assay in CHO Cells with C6-C8 Branched Alkyl Acetate Ester. Project # 164032.

(12) ExxonMobil Biomedical Sciences, Inc. 1997. Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Assay with C6-C8 Branched Alkyl Acetate Ester. Project # 164025.

(13) ExxonMobil Biomedical Sciences, Inc. 2001. Earthworm Acute Toxicity Test. Study # 195992.

(14) ExxonMobil Biomedical Sciences, Inc. 2001. Terrestrial Plant Toxicity Test. Study # 195974.

(15) ExxonMobil Chemical Company (2003). Exxate 700 Data Sheet.

(16) Huntingdon Life Sciences Ltd. 2001. Exxate 700 - Effects on Soil Non-Target Micro-organisms: Nitrogen Transformation, Carbon Transformation. Report No. EXN 031/014049.

(17) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 108419-32-5
CAS No.	:	108419-32-5
TSCA Name	:	Acetic acid, C7-9-branched alkyl esters, C8-rich
Molecular Formula	:	Unspecified

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Status	:	
Memo	:	ExxonMobil HPV
Printing date	:	19.04.2005
Revision date	:	
Date of last update	:	19.04.2005
Number of pages	:	27
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C7-C9 branched alkyl acetate ester

18.12.2000

Exxate 800

07.06.2004

oxo-octyl acetate

07.06.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -30 °C
Sublimation	:	
Method	:	other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no data
Test substance	:	other TS: C8 methyl-branched alkyl acetate ester
Method	:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Remark	:	EPIWIN is used and advocated by the USEPA for chemical property estimation.
Test substance	:	C8 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (9)

2.2 BOILING POINT

Value	:	= 186 - 215 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078 Mod
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (12)

2.3 DENSITY

Type	:	relative density
Value	:	= .87 at 20 °C
Method	:	other: ASTM D891
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (12)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .93 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no data
Test substance	:	other TS: C8 methyl-branched alkyl acetate ester
Test condition	:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Test substance	:	C8 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (9)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 3.66 at 25 °C
pH value	:	
Method	:	other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no data
Test substance	:	other TS: C8 methyl-branched alkyl acetate ester
Test condition	:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	C8 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data

are calculated and not measured.

Flag : Critical study for SIDS endpoint
19.04.2005 (9)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 45 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no data
Test substance	:	other TS: C8 methyl-branched alkyl acetate ester
Test condition	:	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	C8 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (9)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	no
Test substance	:	other TS: C8 methyl-branched alkyl acetate ester
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : CAS No. 108419-32-5; Acetic acid, C7-9 branched alkyl esters, C8-rich
Flag : Critical study for SIDS endpoint
19.04.2005

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000000109403 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance : other TS: C8 methyl-branched alkyl acetate ester

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
11.7	10.94 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : C8 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
19.04.2005 (9)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1998

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 172.27 g/mol
Water solubility = 45 mg/L
Vapour pressure = 93.3 Pa
log Kow = 3.66
Melting point = -30 deg C

Result : Air- 93.3%
Water- 1.3%
Soil- 5.2%
Sediment - 0.1%
Suspended Sed - <0.01%

Biota - <0.01%

Test substance : CAS No. 108419-32-5; Acetic acid, C7-9 branched alkyl esters, C8-rich
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
07.06.2004

(13)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : other: see remark
Exposure period : at °C
Concentration :
BCF : = 151
Elimination :
Method : other: calculation
Year :
GLP : no data
Test substance : other TS: C8 methyl-branched alkyl acetate ester

Remark : A log BCF of 2.2 (BCF = 151) is calculated. C8 methyl-branched alkyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCCCCC(C)CC
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
19.04.2005

(8)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 14.9 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: USEPA 560/6-82-002 Environmental Effects Test Guideline
Year	:	1982
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Result :

96-hour LC50 = 14.9 mg/L (95% CI 9.91 to 20.0) based upon measured TC values.
96-hour LL50 = 49.5 % WAF (95% CI 46.26 to 52.97) based upon nominal values.
Analytical method used was Total Carbon (TC). TC values represent the mean of samples taken on days 0, 2, and 4 less the control value, which was not reported. The LC50 values based upon TC and were re-calculated in 1994 and issued in an amended report.

Measured Conc. (mg/L of TC)	Fish Total Mortality (@96 hrs)*
Control	0
1.39	0
2.71	0
4.90	0
9.91	0
19.86	20

*20 fish added at test initiation
Statistical Method: Probit procedure by Litchfield & Wilcoxon

Test condition :

A stock water accommodated fraction (WAF) was prepared by adding 267ml of the test substance to ~40L of laboratory blend water in a glass carboy. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter and flow-through delivery system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 4.4, 8.8, 17.5, 35.0, and 70.0 % WAF, which measured NA, 1.39, 2.71, 4.90, 9.91, 19.86 mg/L as Total Carbon (TC). The test chambers were glass culture dishes (150 x 75mm). Two replicates with ten fish each were tested per treatment level.
Test temperature was 20.96 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles.
Dilution water hardness was 159 mg/L as CaCO3.
The pH ranged from 7.3 to 8.1. Dissolved Oxygen ranged from 6.7 to 8.4 mg/L.
Fish were supplied by in-house laboratory; age = 13 weeks; mean wt.=0.257g; mean total length=2.4cm; test loading=0.21g of fish/L per 24 hour period.

Reliability : (2) valid with restrictions
Insufficient information in report to assess concentration values.

Flag : Critical study for SIDS endpoint
19.04.2005

(4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	flow through
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 29.4 measured/nominal
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	other: USEPA TSCA
Year	:	1992
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Result :

48 hour EC50 = 29.4 mg (95% CI 24.6 to 36.3) based upon measured TC values.
48 hour EC50 = 73.58 % WAF (95% CI 62.18 to 89.3 %) based upon nominal values.

Analytical method used was Total Carbon (TC). Measured TC values are based upon the mean of samples taken on days 0, 1 and 2 less the control value, which was not reported.

Meas. Conc. (mg TC/L)	Daphnia Total Mortality (@48 hrs)*
Control	1
1.87	1
4.13	1
10.24	0
20.21	3
39.95	17

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.
EC50 based upon TC is the result of a re-calculation in an amended report in 1994.
Statistical Method: Finney, D.J. probit procedure of SAS

Test condition :

A stock water accommodated fraction (WAF) was prepared by combining test substance with laboratory dilution water, at a ratio of 6.7ml per liter of water. The total volume prepared was not reported. The mixture was stirred for 72 hours and the 100% WAF was drawn out via a siphon tube and used for testing. The WAF was administered to the test chambers via a diluter and flow-through delivery system. The diluter system comprised of glass, stainless steel, with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF, which measured: NA, 1.87, 4.13, 10.24, 20.21, and 39.95mg /L as Total Carbon (TC). The test chambers were glass tanks with approximately 6L of test solution flowing through over a 24-hour period. Two replicates with ten daphnids each were tested per treatment level.
Test temperature was 21.36 +/- 0.39 Deg. C. Lighting was 16 hours dark and 8 hour light with gradual on/off periods and an intensity of 83 to 87 ft candles.
Dilution water hardness was 157 mg/L measured as CaCO3.
Dissolved oxygen was 7.9 to 8.8mg/L. The pH ranged from 7.5 to 8.1.

Organisms were supplied by in-house cultures; age = <24 hours old.

Reliability : (2) valid with restrictions
Insufficient information in report to assess concentration values.

Flag : Critical study for SIDS endpoint

19.04.2005 (6)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: USEPA, Environmental Effects Test Guideline EPA 560/6-83-002
Year	:	1983
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Result :

72 hour EL50b=20.97mg TC/L (biomass)
72 hour EL50gr=29.65mg TC/L (growth rate)
96 hour EL50b=19.4mg TC/L (biomass)
96 hour EL50gr=43.52mg TC/L (growth rate)

NOELRb = 31.0 mg/L
NOELRgr = 8.0 mg/L

Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples minus the control value (3.375mg TC/L).
No excursions from the protocol were noted.

Nominal Conc. (%WAF)	Growth Rate 72 & 96 hr. (% Inhibition)		Mean Cell Conc. - 96 hr (cells/ml)
Control	na	na	4.6 x 10(6)
6.25	0.11	1.59	4.0 x 10(6)
12.5	30.24	33.48	2.7 x 10(6)
25.0	2.50	3.33	3.6 x 10(6)
50.0	36.90	34.31	2.5 x 10(6)
100.0	63.51	60.48	1.8 x 10(5)

na - not applicable
Statistical Method: Inverse interpolation method of Snedecor and Cochran

Test condition :

A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1L of algal nutrient media in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separatory funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at 2.0 x 104. The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at ~100 rpm.
The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured, NA, 2.78, 5.74, 10.32, 21.46, and 44.71 mg TC/L respectively.

Test temperature was 23.99 Deg. C. Lighting was continuous at ~4300 Lux (400 ft candles). The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.

Reliability :

(3) invalid
Control TC was 3.3 mg/L instread of the required <2 mg/L.

19.04.2005 (5)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	other: Limit
Value	:	> 3160 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	3
Vehicle	:	other: none
Doses	:	3160 mg/kg
Method	:	other: Experimental (non-regulatory)
Year	:	1983
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)
Result	:	LD50 >3160 mg/kg bw One animal was sacrificed on Day 11 due to severe weight loss. The surviving five animals showed slight weight gain through the study. Dermal evaluations ranged from no erythema to moderate to severe. Edema scores ranged from no edema to slight edema. Desquamation was noted in four animals during the study. The animal terminated on Day 11 revealed kidney discoloration, small spleen, cecum and ileum, and brown material in the stomach. The remaining five animals showed no abnormalities at necropsy.
Test condition	:	Dermal application. Single application / 24-hour occlusive patch. Post dose observation period 14 days. Number of animals per dose per sex = 3. Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14.
Test substance	:	CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)
Conclusion	:	C7-C9 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (3)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	90 days
Frequency of treatm.	:	once/day
Post exposure period	:	
Doses	:	0, 0.1, 0.5, and 1.0 g/kg/day
Control group	:	yes
NOAEL	:	= 1000 mg/kg
Method	:	EPA OTS 798.2650
Year	:	1985
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)
Remark	:	13-Week repeated dose oral toxicity (gavage). Volume: < or = 1.111 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1.111 ml/kg). Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.
Result	:	Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.
Conclusion	:	Oral administration of C7-C9 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical observations were primarily oral and dermal irritation (no clear dose-response). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels for the interim and terminal evaluations. At the terminal sacrifice, there were no biologically significant differences between treated and control animals for the measured clinical chemistries. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. All other organ weights were comparable to control values. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy only in the high-dose male rats that were

consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix, and corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

Reliability : (1) valid without restriction
No circumstances occurred that affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint

19.04.2005 (2)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : other: Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)

System of testing : Bacterial

Test concentration : 25, 50, 100, 200, 400, and 600 µg/plate (25 repeat assay only; 600 initial assay only)

Cycotoxic concentr. :

Metabolic activation : with and without

Result : negative

Method : EPA OPP 84-2

Year : 1994

GLP : yes

Test substance : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Remark : Species/Strain - S. typhimurium / TA98, TA100, TA1535, TA1537, TA1538

Species/cell type - Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9)

Vehicle - DMSO

Result : C7-C9 branched alkyl acetate ester, did not induce significant increases in revertant colonies (> 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either a reduction in the number of revertant colonies or a reduction in the background lawn, was observed for all five tester strains with an without metabolic activation in both the initial and repeat assays, except for tester strain TA1535 with metabolic activation for the repeat assay. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

Test condition : There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 25, 50, 100, 200, 400, or 600 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar,

vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 °C for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

Test substance : CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Conclusion : C7-C9 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint

19.04.2005 (11)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : other: In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method

Species : mouse

Sex : male/female

Strain : other: Crl:CD-1 (VAF/Plus)

Route of admin. : gavage

Exposure period : 24, 48 and 72 hours

Doses : 0.625, 1.25, and 2.5 grams/kg / Single dose

Result : negative

Method : EPA OTS 798.5395

Year : 1994

GLP : yes

Test substance : other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Result : A statistically significant increase in the mean number of micronucleated polychromatic erythrocytes was not seen at any dose level. Cytotoxicity, shown by a dose-related decrease in the percentage of polychromatic erythrocytes, was observed for both sexes at the 48-hour sampling time (regression coefficient $p<0.01$). The two highest dose groups were statistically different from the vehicle control. Both the positive (cyclophosphamide) and negative (vehicle carrier) controls responded in an appropriate manner.

The test material is considered to be toxic to bone marrow in CD-1 mice under the conditions of this test based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

Test condition : Vehicle: Corn Oil

Positive Control: Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage

The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei

(1000 polychromatic erythrocytes/animal were evaluated).

Test substance	:	CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)
Conclusion	:	C7-C9 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (10)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gravid day 6-15
Frequency of treatm.	:	single dose daily
Duration of test	:	Gravid day 20
Doses	:	0, 100, 500 and 1000 mg/kg
Control group	:	other: Sham-Treated with distilled water at 1000 mg/kg
NOAEL maternal tox.	:	500 mg/kg bw
NOAEL teratogen.	:	500 mg/kg bw
other: NOEL Maternal	:	100 mg/kg bw
other: NOEL Pup	:	500 - mg/kg bw
Method	:	EPA OTS 798.4900
Year	:	1985
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-32-5; Acetic acid, C7-9 methyl-branched alkyl esters, predominantly C8 (>90%)

Remark : Developmental Toxicity with 22 mated female Sprague-Dawley rats per dose. Vehicle: none.

For the 1000 mg/kg group, there was a slightly increased incidence of malformations, although the different types of malformations, observed did not suggest a characteristic pattern of anomalies. No developmental toxicity was observed at the maternally toxic dose of 500 mg/kg or the maternally nontoxic dose of 100 mg/kg.
Statistical Methods: Maternal body weight, body weight change, food consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-

significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.

Conclusion : C7-C9 branched alkyl acetate ester, was administered at 0, 100, 500, and 1000 mg/kg on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen at the 500 and 1000 mg/kg doses as evidenced by decreases in body weight and food consumption. There was a slight, but not significant increase in fetal malformations and embryotoxicity in the 1000 mg/kg group only; no adverse fetal effects were observed in the 100 and 500 mg/kg groups. (Daughtrey, et al., 1989)

Reliability : (1) valid without restriction
No circumstances occurred that affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint

19.04.2005 (1) (7)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bio/Dynamics Inc., East Millstone, NJ, Oral Teratology Study in Rats Project # 330334.

(2) Bio/dynamics Inc., East Millstone, NJ, Subchronic Oral Gavage Study in Rats; Project # 230370.

(3) Bio/dynamics Inc., East Millstone, NJ, USA, Acute Dermal Toxicity Study in the Rabbit with C7-C9 Branched Alkyl Acetate Ester. Project # 330306.

(4) BioDynamics Inc. 1985. A Flow-Through Acute Fish Toxicity Test. Study #230341.

(5) BioDynamics Inc. 1985. Algal Acute Toxicity Test. Study #230359.

(6) BioDynamics, Inc. 1985. A Flow-Through Acute Daphnia Toxicity Test. Study # 230364.

(7) Daughtrey W, Wier P, Traul K, Biles R and Egan G (1989). Evaluation of the teratogenic potential of octyl acetate in rats. Fund. Appl. Toxicol. 13:202-309.

(8) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(9) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(10) Exxon Biomedical Sciences, Inc. 1994. In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method with C7-C9 Branched Alkyl Acetate Ester. Project # 168830.

(11) Exxon Biomedical Sciences, Inc., 1994. Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay with C7-C9 Branched Alkyl Acetate Ester. Project # 168825.

(12) ExxonMobil Chemical Company (2003). Exxate 800 Data Sheet.

(13) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-16018

I U C L I D

Data Set

05 AUG 31 PM 2:22

Existing Chemical	:	ID: 108419-33-6
CAS No.	:	108419-33-6
TSCA Name	:	Acetic acid, C8-10-branched alkyl esters, C9-rich
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Status	:	
Memo	:	ExxonMobil HPV
Printing date	:	19.04.2005
Revision date	:	
Date of last update	:	19.04.2005
Number of pages	:	21
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C8-C10 branched alkyl acetate ester

07.06.2004

Exxate 900

07.06.2004

oxo-nonyl acetate

07.06.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -20 °C
Sublimation	:	
Method	:	other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C13 methyl-branched alkyl acetate ester
Method	:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Remark	:	EPIWIN is used and advocated by the USEPA for chemical property estimation.
Test substance	:	C13 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (4)

2.2 BOILING POINT

Value	:	= 205 - 235 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078 Mod
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

07.06.2004 (5)

2.3 DENSITY

Type	:	relative density
Value	:	= .87 at 20 °C
Method	:	other: ASTM D891
Year	:	
GLP	:	no data
Test substance	:	other TS

Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

07.06.2004 (5)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .35 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)
Test condition	:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Test substance	:	CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 4.15 at 25 °C
pH value	:	
Method	:	other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)
Test condition	:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters,

predominantly C9 (>75%)

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
19.04.2005 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 14.5 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)
Test condition	:	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, predominantly C9 (>75%)
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	
Test substance	:	other TS: C9 methyl-branched alkyl acetate ester
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : CAS No. 108419-33-6; Acetic acid, C8-10 branched alkyl esters, C9-rich
Flag : Critical study for SIDS endpoint
19.04.2005

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000000123533 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance : other TS: C9 methyl-branched alkyl acetate ester

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
10.4	12.35 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : C9 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
19.04.2005 (4)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1998

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 186.3 g/mol
Water solubility = 14.5 mg/L
Vapour pressure = 34.7 Pa
log Kow = 4.15
Melting point = -20 deg C

Result : Air- 86.7%
Water- 1.0%
Soil- 12.1%
Sediment - 0.3%
Suspended Sed - <0.01%

Biota - <0.01%

Test substance : C9 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
19.04.2005 (6)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species : other: see remark
Exposure period : at °C
Concentration :
BCF : = 316
Elimination :
Method : other: calculation
Year :
GLP : no data
Test substance : other TS: C9 methyl-branched alkyl acetate ester

Remark : A log BCF of 2.5 (BCF = 316) is calculated. C9 methyl-branched alkyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCC(C)CCC(C)CC
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
19.04.2005 (3)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	other: Limit
Value	:	> 5000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: None
Doses	:	
Method	:	other:Experimental
Year	:	1983
GLP	:	yes
Test substance	:	other TS:C8-C10 branched alkyl acetate ester
Remark	:	There was one female death on day 4 during this study. Nine of 10 animals showed staining in the ano-genital area on Day 1 and all 10 showed staining on Day 2. Hypopnea was observed in 3 rats on Day 1. Other clinical observations included unthrifty coat, hypoactivity, prostration, urinary staining, and soft stool in the first 4 days. Alopecia was observed in one female from Day 10 through 14. All surviving animals showed an increase over pre-dose weights. Five of 9 surviving animals showed no observable abnormalities during postmortem examination. Three animals showed lung discoloration typical of findings resulting from carbon dioxide asphyxiation. The animal that succumbed prior to study termination exhibited vascularization and distension of the cecum; thickened amber material present in the duodenum; thickened red material in the jejunum; an accentuated lobular pattern present in the liver; and, a slightly reddened thymus.
Conclusion	:	C8-C10 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered orally. Signs of slight toxicity were limited to the first 4 days.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

11.12.2001 (2)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	other: Limit
Value	:	> 3160 - mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	3
Vehicle	:	other: none
Doses	:	3160 mg/kg
Method	:	other: Experimental (Non-regulatory)
Year	:	1983

GLP	:	yes
Test substance	:	other TS
Result	:	LD50 >3160 mg/kg bw Erythema was noted in all animals at 24 hours and continued in four animals through Day 14. Edema was seen in three animals at 24 hours. No animals showed edema by the Day 7 evaluation. Desquamation was seen in one animal on Day 7, three animals on Day 10 and remained in two animals at the Day 14 termination. One male and two females at Day 7 and one male and one female showed slight decreases in body weight. Food consumption was reduced on Day 1 only. Postmortem examination revealed gallbladder and salivary gland abnormalities, kidney discoloration, a urinary bladder abnormality, hair in two stomachs and ano-genital staining.
Test condition	:	Dermal Application, Single application / 24-Hour Occlusive Patch, Post Dose Observation Period 14 Days. Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14.
Test substance	:	CAS No. 108419-33-6, C8-C10 branched alkyl acetate ester
Conclusion	:	C8-C10 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin at 3160 mg/kg.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

02.03.2004 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bio/dynamics Inc. 1983. Acute Dermal Toxicity Study in the Rabbit with C8-C10 Branched Alkyl Acetate Ester. Project # 330406.

(2) Bio/dynamics, East Millstone, NJ, Acute Oral Toxicity Study in the Rat; Project # 330401.

(3) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(4) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(5) ExxonMobil Chemical Company (2003). Exxate 900 Data Sheet.

(6) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-16018

I U C L I D

Data Set

05 AUG 31 PM 2:22

Existing Chemical	:	ID: 108419-34-7
CAS No.	:	108419-34-7
TSCA Name	:	Acetic acid, C9-11-branched alkyl esters, C10-rich
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Status	:	
Memo	:	ExxonMobil HPV
Printing date	:	19.04.2005
Revision date	:	
Date of last update	:	19.04.2005
Number of pages	:	23
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C9-C10 branched alkyl acetate ester

07.06.2004

Exxate 1000

07.06.2004

oxo-decyl acetate

07.06.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -8.8 °C
Sublimation	:	
Method	:	other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C10 methyl-branched alkyl ester
Method	:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Remark	:	EPIWIN is used and advocated by the USEPA for chemical property estimation.
Test substance	:	C10 methyl-branched alkyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (3)

2.2 BOILING POINT

Value	:	= 220 - 250 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078 Mod
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	CAS No. 108419-34-7; Acetic acid, C9-11 methyl-branched alkyl esters, predominantly C10 (>85%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

07.06.2004 (7)

2.3 DENSITY

Type	:	relative density
Value	:	= .87 at 20 °C
Method	:	other: ASTM D891
Year	:	
GLP	:	no data

Test substance	:	other TS: CAS No. 108419-34-7; Acetic acid, C9-11 methyl-branched alkyl esters, predominantly C10 (>85%)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (7)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .13 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C10 methyl-branched alkyl esters
Test condition	:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation.
Test substance	:	C10 methyl-branched alkyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 4.65 at 25 °C
pH value	:	
Method	:	other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS
Test condition	:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	C10 methyl-branched alkyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

07.06.2004 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 4.7 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C10 methyl-branched alkyl ester
Test condition	:	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	C10 methyl-branched alkyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	no
Test substance	:	other TS: C10 methyl-branched alkyl ester
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : C10 methyl-branched alkyl ester
Flag : Critical study for SIDS endpoint
19.04.2005

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000000137664 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance : other TS: C10 methyl-branched alkyl ester

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
9.3	13.76 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : C10 methyl-branched alkyl ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
19.04.2005 (3)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1998

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 200.32 g/mol
Water solubility = 4.7 mg/L
Vapour pressure = 13.3 Pa
log Kow = 4.65
Melting point = -8.8 deg C

Result : Air- 73.4%
Water- 0.6%
Soil- 25.3%
Sediment - 0.6%
Suspended Sed - 0.02%

Biota - <0.01%

Test substance : C10 methyl-branched alkyl ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
19.04.2005 (8)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic
Contact time : 28 day(s)
Degradation : = 84.7 (±) % after 28 day(s)
Result :
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 1993
GLP : yes
Test substance : other TS: C10 methyl-branched alkyl ester

Result : Test material was readily biodegradable. Half-life was 1 week. By day 28, 85% degradation of the test material was observed. 10% biodegradation was achieved on day 2, 50% biodegradation on approximately day 7. By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted.
Biodegradation was based on oxygen consumption and the theoretical oxygen demand (ThOD) of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	81, 92, 81	84.7
Na Benzoate	92, 91	91.5

* replicate data

Test condition : Test vessels were electronically monitored for oxygen consumption. Test material was tested in triplicate, while controls and blanks were tested in duplicate.
Test material concentration was approximately 45mg/L. Sodium benzoate (positive control) concentration was 50mg/L.
The inoculum was not acclimated.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
Reliability : (2) valid with restrictions
Data were provided in a summary report, in which details of treatment preparation, media, vessel size, and temperature were not reported. However, the test procedure followed the OECD 301F test guideline.
Flag : Critical study for SIDS endpoint
19.04.2005 (4)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at °C
Concentration	:	
BCF	:	= 754
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no data
Test substance	:	other TS: C10 methyl-branched alkyl acetate ester
Remark	:	A log BCF of 2.9 (BCF = 754) is calculated. C10 methyl-branched alkyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCC(C)CCCC(C)CC
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (2)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	1984
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-34-7; Acetic acid, C9-11 methyl-branched alkyl esters, predominantly C10 (>85%)

Result :

48 hour EL50 = 6.7 mg/L (95% CI 5.1 to 8.8) based upon nominal values

48 hour EC50 = 1.8 mg/L (95% CI 1.3 to 2.3) based upon measured values (not in report)

Analytical method used was GC-MSD. Measured values are based upon the mean of samples taken on day 0, and day 2.

Nominal. Conc. (mg/L)	Daphnia Total Immobility (@48 hrs)*
Control	0
1.3	0
3.2	4
8.0	11
20.0	19
50.0	20

*20 Daphids total added at test initiation.
Mortality is defined as immobilized.
Statistical Method: Trimmed Spearman Karber

Test condition : Individual treatment solutions were prepared as water accommodated fractions (WAFs). A WAF was prepared by adding test substance, via syringe, to 2.0L of laboratory dilution water in a glass aspirator bottle and mixing with a magnetic stir plate and bar. Mixing vortex was <10% of solution volume. After mixing for 24 hours at room temperature, the WAF was allowed to settle for one hour and removed from the port at the bottom of the bottle.
Test vessels were 125ml glass beakers filled with 140ml of solution and covered (no headspace). Four replicates were prepared for each treatment. Each replicate contained 5 organisms.
Nominal treatment levels were; control, 1.3, 3.2, 8.0, 20.0, and 50.0mg/ which measured; ND, 0.44, 1.3, 2.1, 1.9, 2.2mg/L respectively.
Test temperature was 20.0 Deg C. Lighting measured 691 Lux with 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 6.8 to 8.3mg/L. The pH ranged from 7.2 to 7.6.

Organisms were supplied by in-house cultures; age = <24 hours old. Parents age = 15 days old.

Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005

(5)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: Pseudokirchneriella subcapitata
Endpoint	:	other: growth rate / biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
EL50 (biomass)	:	> 1021 measured/nominal
EL50 (growth rate)	:	> 1021 measured/nominal
NOEL	:	= 254 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: OECD 201 and EU Directive 92/69/EEC part C3
Year	:	2003
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-34-7; Acetic acid, C9-11 methyl-branched alkyl esters, predominantly C10 (>85%)

Result :

72 hour EL50 >1021 mg/L (biomass and growth rate) based on nominal values

72 hour NOEL = 254 mg/L (biomass and growth rate) based on nominal values

The very wide range of loading levels, and low level and narrow range of measured values precluded the use of the measured values for statistical analysis. Therefore, the results are presented corresponding to test substance loading level and not test substance concentration. Samples of the test substance in water were extracted with hexane and analyzed by gas chromatography with flame ionization detection (GC-FID).

Mean Cell Density

Nominal Conc. (mg/L)	(% inhibition) (growth)	(cells/ml)
Control	n/a	1.7x10(7)
64.5	13.0	1.4x10(6)
130	8.0	1.5x10(6)
254	8.9	1.5x10(6)
522	16.0	1.4x10(6)
1021	16.0	1.4x10(6)

n/a = not applicable

Statistical method: PROC regression procedure of SAS, ANOVA procedure of SAS for NOEL.

Test condition : Individual treatments were prepared as Water Accommodated Fractions (WAFs) by adding the appropriate amount of test substance to algal nutrient media in glass aspirator bottles and stirring on magnetic stirplates for approximately 24.5 hours. The mixtures were allowed to settle for approximately 1 hour before removing the aqueous portions (WAFs) for testing.

The test substance actual loading levels for this study were 64.5, 130, 254, 522, and 1021 mg/L. The measured test substance concentrations at the start of the study were 4.80, 5.00, 5.22, 5.24, and 5.57 mg/L, respectively. A control treatment consisting of algal nutrient media (dilution water) with no test substance was also tested.

Four replicate chambers were established for each treatment and the control. The mouths of the test chambers were covered with foam stoppers. Test chambers were placed on a shaker table (at 100 oscillations/minute) to keep the algae in suspension. The study was performed under continuous light conditions (7600 - 7700 Lux) at approximately 22°C. The pH was recorded on the test solutions at the beginning and end of the test. The pH ranged from 7.4 to 7.5 at the start of the test, and from 7.1 to 7.2 at the end of the test. Cell counts were performed daily on each replicate.

The initial algal concentration was 1.0x10(4) cells/ml.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
19.04.2005

(6)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	other: Limit
Value	:	> 3160 - mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	3
Vehicle	:	other: none
Doses	:	3160 mg/kg bw
Method	:	other: Experimental (Non-regulatory)
Year	:	1984
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-34-7; Acetic acid, C9-11 methyl-branched alkyl esters, predominantly C10 (>85%)
Result	:	LD50 >3160 mg/kg bw There were no deaths during the course of this study. Three of six animals gained weight during the study. Clinical in-life observations included ano-genital staining, ocular discharge, unthrifty coat, nasal discharge and poor food consumption. Erythema and edema were slight to well defined. Desquamation was also observed. Postmortem examination revealed kidney discoloration, an encapsulated salivary gland, an enlarged cervical lymph node and hair present in the stomach.
Test condition	:	Single dermal application / 24-Hour Occlusive Patch, Post Dose Observation Period 14 Days. Clinical observations were made 2, 4 and 24 hours after dosing and on days 3, 7, 10 and 14 according to the Draize method of scoring. Body weights were recorded on the day of dosing, on Day 7 and on Day 14. Gross necropsies were performed on Day 14.
Test substance	:	CAS No. 108419-34-7; Acetic acid, C9-11 methyl-branched alkyl esters, predominantly C10 (>85%)
Conclusion	:	C9-C11 branched alkyl acetate ester has a low order of percutaneous toxicity when administered in a single dose to intact rabbit skin at 3160 mg/kg bw.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bio/dynamics Inc. 1984. Acute Dermal Toxicity Study in the Rabbit with C9-C11 Branched Alkyl Acetate Ester. Project # 330506.

(2) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(3) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(4) Exxon Biomedical Sciences Inc. 1996. Ready Biodegradability, Manometric Respirometry. Study #129794A.

(5) Exxon Biomedical Sciences, Inc. 2000. Daphnia Acute Immobilization Test. Study #129942.

(6) ExxonMobil Biomedical Sciences Inc. 2003. Alga, Growth Inhibition Test. Study #145767.

(7) ExxonMobil Chemical Company (2003). Exxate 1000 Data Sheet.

(8) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	ID: 108419-35-8
CAS No.	:	108419-35-8
TSCA Name	:	Acetic acid, C11-14-branched alkyl esters, C13-rich
Molecular Formula	:	Unspecified
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	07.12.2000
Status	:	
Memo	:	ExxonMobil HPV
Printing date	:	19.04.2005
Revision date	:	
Date of last update	:	19.04.2005
Number of pages	:	30
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the alkyl acetates category.

Remark : Alkyl Acetates follow a regular pattern as a result of synthesis and structural similarity. Aliphatic, monohydric alcohols are reacted with acetic acid to form the corresponding acetate esters (CH3COOR).
Members associated with this template category are:
88230-35-7 Hexanol, acetate, branched and linear
90438-79-2 Acetic acid, C6-8 branched alkyl esters
108419-32-5 Acetic acid, C7-9 branched alkyl esters
108419-33-6 Acetic acid, C8-10 branched alkyl esters
108419-34-7 Acetic acid, C9-11 branched alkyl esters
108419-35-8 Acetic acid, C11-14 branched alkyl esters

07.12.2000

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

C11-C14 branched alkyl acetate ester

18.12.2000

Exxate 1300

07.06.2004

oxo-tridecyl acetate

07.06.2004

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -2 °C
Sublimation	:	
Method	:	other: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C13 methyl-branched alkyl acetate ester
Method	:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Remark	:	EPIWIN is used and advocated by the USEPA for chemical property estimation.
Test substance	:	C13 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (12)

2.2 BOILING POINT

Value	:	= 240 - 285 °C at 1013 hPa
Decomposition	:	
Method	:	other: ASTM D1078 Mod
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)
Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (16)

2.3 DENSITY

Type	:	relative density
Value	:	= .87 at 20 °C
Method	:	other: ASTM D891
Year	:	
GLP	:	no data
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Reliability	:	(4) not assignable This robust summary has a reliability rating of 4 because the data were not retrieved and reviewed for quality.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (16)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .013 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C13 methyl-branched alkyl acetate ester
Test condition	:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation.
Test substance	:	C13 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (12)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 6.05 at 25 °C
pH value	:	
Method	:	other (calculated): Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C13 methyl-branched alkyl acetate ester
Test condition	:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.
Test substance	:	C13 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (12)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= .2 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year	:	1999
GLP	:	no
Test substance	:	other TS: C13 methyl-branched alkyl acetate ester
Test condition	:	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.
Test substance	:	C13 methyl-branched alkyl acetate ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (12)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): Technical Discussion
Year	:	
GLP	:	no
Test substance	:	other TS: C13 methyl-branched alkyl acetate ester
Remark	:	These data represent a key study for characterising the potential of substances in the Alkyl Acetates C6 to C13 category to undergo direct photodegradation.
Result	:	Photolysis as a Function of Molecular Structure

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Substances in the Alkyl Acetate C6 to C13 Category contain molecules that are oxygenated aliphatic compounds which will absorb only in the far UV region, below 220 nm, (Boethling and Mackay, 2000) and therefore will not undergo direct photolysis. These data indicate that photolysis will not significantly contribute to the degradation of alkyl acetate esters in the aquatic environment.

References

Boethling, R.S., Mackay, D. (2000). Handbook of Property Estimation Methods for Chemicals. CRC Press, Boca Raton, FL, USA.

Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York,

USA.

Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

Test substance : C13 methyl-branched alkyl acetate ester
Flag : Critical study for SIDS endpoint
19.04.2005

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000000186925 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated): Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year : 1999
GLP : no
Test substance : other TS: C13 methyl-branched alkyl acetate ester

Result : Atmospheric Oxidation Potential

In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993).

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Calculated* half-life (hrs)	OH- Rate Constant (cm3/molecule-sec)
6.9	18.69 E-12

References:

Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environ. Toxicol. Chem. 7:435-442.

Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 12:2293-2299.

Test condition : Indirect photodegradation, or atmospheric oxidation potential, is based on

the structure-activity relationship methods developed by R. Atkinson.

Temperature: 25°C
Sensitizer: OH radical
Concentration of Sensitizer: 1.5 E6 OH radicals/cm3

Test substance : C13 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for the test substance.
Flag : Critical study for SIDS endpoint
19.04.2005 (12)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1998

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program. Measured input values were also used where available and obtained from the EPIWIN database. Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Input values used:
Molecular mass = 242.41 g/mol
Water solubility = 0.2 mg/L
Vapour pressure = 1.33 Pa
log Kow = 6.05
Melting point = -2 deg C

Result : Air- 24.2%
Water- 0.07%
Soil- 74.0%
Sediment - 1.6%
Suspended Sed - 0.05%

Biota - <0.01%

Test substance : C13 methyl-branched alkyl acetate ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
19.04.2005 (17)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other: acclimated inoculum
Contact time : 28 day(s)
Degradation : = 31 (±) % after 28 day(s)
Result :
Deg. product :
Method : other: USEPA EPA 560/6-83-003, CG-2000 Aerobic Aquatic Biodegradation Test
Year : 1982
GLP : yes
Test substance : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Result : By day 28, 31% degradation of the test material was observed. The half-life, and 10% biodegradation achievement periods were not reported. The positive control (phthalic acid) degraded by 43.8% by day 28, with a TOC removal of 100.7%. TOC was not measured for the test material. The negative control, HgCl2, showed no activity. Biodegradation was based on CO2 evolution. No excursions from the protocol were noted.

Test condition : The inoculum was acclimated to the test substance for 14 days prior to study initiation. The media consisted of mineral salt solutions, pond sediment, activated sludge, distilled water, and small amounts (10ul) of test substance. The media was mixed and placed on a gyrorotatory shaker in the dark for 13 days. After settling overnight the supernatant was pour off and was used as the inoculum for the test phase.

The test system utilized 2.0L Glenhill flasks as test vessels. Approximately 13.0 mg (9.6 mg carbon) of test substance was added to 900ml of glass distilled water. Additionally, 100ml of acclimated media and 1ml of mineral salts were added. The flasks were sealed and placed on a gyrorotatory shaker in the dark. Three replicates of the test substance were evaluated. Twice a week, the flasks were monitored for spent NaOH and titrated for carbon dioxide (CO2). Total Organic Carbon (TOC) was measured at initiation and termination in the controls.

A positive and negative control were tested consisting of Phthalic acid (100ml at 103.8mg/L) and HgCl2 (10 ml at 51g/L) respectively, along with three blanks.

Test temperature ranged from 21.5 to 25.0 Deg C.

Reliability : (2) valid with restrictions
TOC values not measured on test treatments only controls. No replicate values reported (mean values only).
Flag : Critical study for SIDS endpoint
19.04.2005 (10)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	other: see remark
Exposure period	:	at °C
Concentration	:	
BCF	:	= 325
Elimination	:	
Method	:	other: calculation
Year	:	
GLP	:	no data
Test substance	:	other TS: C13 methyl-branched alkyl acetate ester
Remark	:	A log BCF of 2.5 (BCF = 325) is calculated. C13 methyl-branched alkyl acetate ester in the aquatic environment is expected to have a low potential for bioaccumulation. The SMILES notation used was CC(=O)OCC(C)CCCCCCC(C)CC
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (11)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LL0	:	= 5800 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: USEPA 40 CFR 792
Year	:	1984
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Result : 96 hour LL0 = 5800 mg/L based upon nominal loading levels. There was no mortality at saturation.

The amount of TC (total carbon) measured (less the control value) in the exposure solutions was below detection limit.

Nominal Conc. (% WAF)	Fish Total Mortality (@96 hrs)*
Control	0
6.25	0
12.5	0
25.0	0
50.0	0
100.0	0

*20 fish added at test initiation
The analytical method measured Total Carbon (TC). TC was monitored in exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TC for each level tested. No significantly high or low levels were seen.

Test condition : A stock water accommodated fraction (WAF) was prepared by adding the test substance to laboratory blend water at a ratio of 1:150. The solution was stirred for 72 hours and the 100% WAF used for testing. The WAF was administered to the test chambers via a diluter system. The diluter system comprised of glass, stainless-steel with no plasticized materials. The diluter prepared the following test treatment levels: control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF. The test chambers were 15L glass tanks containing 14L of solution. Two replicates with ten fish each were tested per treatment level.
Test temperature was 21.78 +/- 0.15 Deg C. Lighting was gradual on and off with 16 hours dark and 8 hour light with an intensity of 77 to 79 ft candles.
Dilution water hardness was 158 mg/L as CaCO3.
The pH ranged from 7.6 to 8.0. Dissolved Oxygen ranged from 7.7 to 8.6 mg/L.
Fish were supplied by in-house laboratory; age = 25 weeks; mean wt.=0.276g; mean total length=2.5cm; test loading=0.023g of fish/L per 24 hour period.

Conclusion	:	The test material is considered non-toxic at its level of water solubility.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (8)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EL0	:	= 5829 measured/nominal
Limit Test	:	no
Analytical monitoring	:	yes
Method	:	other: USEPA 560/6-82
Year	:	1984
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Result : 48 hour EL0 = 5829 mg/L based upon nominal loading levels. There was no immobility at saturation.

Nominal. Conc. (% WAF)	Daphnia Total Immobility (@48 hrs)*
Control	0
6.25	0
12.5	0
25.0	0
50.0	0
100.0	0

*40 Daphids total added at test initiation.
Mortality is defined as immobilized.
Some daphnids observed swimming on the surface in all treatment levels.

Three trials of the study were performed to confirm study results. Trials 2 and 3 exhibited no toxicity (trial 1 was not reported). The third trial is documented here.
Analytical method used was Total Carbon (TC). The measured TC values (less the controls) were within the variability of the analytical method. TC was monitored in exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TC for each level tested. No significantly high or low levels were seen.

Test condition : A water accomodated fraction (WAF) was prepared as a stock solution and then diluted to prepare the individual treatment levels. The WAF was prepared by adding 16.75ml of the test substance to 2.5L of laboratory dilution water in a glass carboy and mixed with a magnetic stir plate and bar. After mixing for 72 hours, the 100% WAF was drawn out through a sampling tube.
Test vessels were 400ml glass beakers filled with 250ml of solution and covered. Four replicates were prepared for each treatment. Each replicate contained 10 organisms.
Nominal treatment levels were; control, 6.25, 12.5, 25.0, 50.0, and 100.0 % WAF.
Test temperature was 20.92 Deg C. Lighting measured 78 to 85 ft. candles with 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.3 to 9.5mg/L. The pH ranged from 8.2 to 8.5 units.

Organisms were supplied by in-house cultures; age = <24 hours old.
Parents age = 13 days old.

Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (13)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
Limit test	:	no
Analytical monitoring	:	yes
Method	:	other: USEPA, EPA 560/6-83-002
Year	:	1983
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Result :

96 hour EL0b: = 5829 mg/L based upon calculated laoding level.
96 hour EL0gr: = 5829 mg/L based upon calculated loading level.
There was no inhibition at saturation.

NOELRb = 5829 mg/L based upon nominal loading levels.
NOELRgr= 5829 mg/L based upon nominal loading levels.

No Inhibition of Algal growth was observed at the highest treatment level 100% WAF (0.873 ppm Carbon)

Nominal Conc. (%WAF)	Mean Cell Conc. - 96 hr (cells/ml)
Control	5.2x10(6)
6.25	4.4 x10(6)
12.5	4.6 x10(6)
25.0	4.1 x10(6)
50.0	5.3 x10(6)
100.0	5.2 x10(6)

Analytical method used was Total Carbon (TC). Measured TC values are based upon Day 0 samples less the control value on day 0 of the study. TC was monitored in exposure solutions and the control to identify solutions that exhibited unexplainably high or low levels of TC for each level tested. No significantly high or low levels were seen.

No excursions from the protocol were noted.

Test condition : A Water Accommodated Fraction (WAF) stock solution was prepared by adding 6.7ml of test substance to 1L of algal nutrient media (AAP) in a 2L flask and mixed slowly for 72 hours. After mixing, the solution was transferred to a separatory funnel and allowed to settle for one hour. After settling, the solution was removed from the bottom and used as the 100% WAF. Individual treatments were prepared by diluting the 100% WAF with algal nutrient media. The test treatments were divided into 4 replicates. Three replicate were inoculated with algae at 2.0 x 104. The remaining replicate served as a blank. Treatment replicates were 125 ml erlenmeyer flasks containing 50 ml of solution. Flasks were placed on a shaker table during the study at ~100 rpm.
The test treatment concentrations were; control, 6.25, 12.5, 25, 50 and 100% WAF which measured (less the control value) na, 0, 0.058, 0.219, 0.492, and 0.873ppm of TC.

Test temperature was 23.89 Deg. C. Lighting was continuous at 400 ft candles. The pH was 7.5 at test initiation and ranged from 7.3 to 7.4 at test termination.

Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

19.04.2005 (9)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	other: Limit
Value	:	> 5000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: none
Doses	:	5.721 ml/kg
Method	:	other: Experimental
Year	:	1983
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)
Remark	:	Route of Administration: oral gavage. Number of animals per dose per sex = 5. Single (18-hr fasted) dose of 5.721 ml/kg (1.1-1.9 ml). Post dose observation period of 14 days. There were no deaths during this study. Nine of 10 animals showed staining in the ano-genital area on Days 1 and 2, and for 1 animal on Day 3. Soft stool was noted for 1 animal at 6 Hrs PD and white gelatinous material on the penis was noted for 1 animal on Day 1. There were no observable abnormalities noted after the Day 3 observations. All animals except one showed an increase over pre-dose weights except one animal that appeared to have had an incorrect pre-dose weight recorded. Six of 10 animals showed no observable abnormalities during postmortem examination. Four animals showed lung discoloration typical of findings resulting from carbon dioxide asphyxiation.
Conclusion	:	C11-C14 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered orally. Signs of slight toxicity (staining of the fur and soft stool) were limited to the first 3 days.
Reliability	:	(1) valid without restriction No Circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (7)

Type	:	other: Repeated-Dose Probe
Value	:	> 3000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: none
Doses	:	0, 0.1, 0.5, 1.0, or 3.0 g/kg
Method	:	other: Experimental
Year	:	1985
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)
Remark	:	Route of Administration: oral gavage. Number of animals per dose per sex = 4. Doses / time: 0, 0.1, 0.5, 1.0, or 3.0 g/kg / Once daily for a total of

9 doses. Vol. Admin.: < or = 3.333 ml/kg. Post dose observation period of 11 days.

One control animal was euthanized on Day 7 due to a moribund condition following a caging accident. All other animals survived to study termination and exhibited increases in body weight. In-life clinical observations showed no observable abnormalities throughout the study period for the surviving control animals and the majority of those dosed with 0.1, 0.5, or 1.0 g/day. The animals dosed with 3.0 g/day showed scattered incidences of wet rales, protruding penis, urinary and fecal staining, and soft stool; for the majority of the test period they showed no observable abnormalities. As a group, only the 0.1 males showed decreases in mean hematocrit and hemoglobin compared to controls (values for 2 animals were significantly lower than all other animals). Females showed significant decreases in mean red blood cell count, hematocrit, and hemaglobin values compared to controls. Gross postmortem examination showed dilated renal pelvis for 1 control and 1 animal of the 1.0 g/day dose group. A large discolored ovary was observed in a 0.1 g/day animal and a thymic discoloration was seen in a 0.5 g/day animal. Two animals at the 3.0 g/day dose level showed staining of the ano-genital area.

Conclusion : C11-C14 branched alkyl acetate ester elicited minimal signs of acute systemic toxicity when administered once daily for a total of 9 doses by oral gavage.

Reliability : (1) valid without restriction
No Circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint
19.04.2005 (3)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : other: Limit
Value : > 3160 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 3
Vehicle : other: none
Doses : 3160 mg/kg bw
Method : other: Experimental (Non-regulatory)
Year : 1984
GLP : yes
Test substance : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Remark : Route of Administration: dermal application. Number of animals per dose per sex = 3. Single application / 24-hour occlusive patch of 3160 mg/kg. Post dose observation period of 14 days.

There were no overt signs of systemic toxicity. Five of 6 rabbits showed slight body weight decreases at Day 7; only 2 animals continued to have decreased body weight at 14 days. Slight dermal irritation persisted in 4 of 6 test animals through termination of the study. In general, dermal responses were considered minimal and transient in nature. At post mortem examination, 3 of 6 animals showed no observable abnormalities. Liver and salivary gland discoloration was observed in one animal; kidney

discoloration and spleen enlargement in another; and alopecia in the third animal.

Conclusion : C11-C14 branched alkyl acetate ester did not elicit signs of percutaneous toxicity when administered to intact rabbit skin.

Reliability : (1) valid without restriction
No Circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint

19.04.2005 (2)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : .5 other: ml
Exposure : Semiocclusive
Exposure time : 4 hour(s)
Number of animals : 6
Vehicle :
PDII : .67
Result :
Classification :
Method : EPA OTS 798.4470
Year : 1983
GLP : yes
Test substance : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Remark : Route of Administration: dermal application. Number of animals per dose per sex = 3. Single application / 4-hour semi-occlusive patch of 0.5 ml. Post dose observation period 1, 24, 48, and 72 hours and Day 7.

All animals survived to study termination, were free of clinical signs, and 5 of 6 animals displayed an increase in body weight during the test period. All animals showed erythema in the first 72 hours. The mean score for erythema was 0.67. One of 6 animals showed very slight erythema at the day 7 observation. The study was terminated on Day 7.

Result : mild dermal irritant to rabbit skin.

Conclusion : C11-C14 branched alkyl acetate ester is a mild dermal irritant to rabbit skin.

Reliability : (1) valid without restriction
No Circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint

19.04.2005 (5)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : 100 %
Dose : .1 ml
Exposure time :
Comment :
Number of animals : 3
Vehicle : none
Result :
Classification :

Method	:	EPA OTS 798.4500
Year	:	1983
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)
Remark	:	Draize Ocular Irritation on male and female New Zealand White rabbits. Number of animals per dose per sex = 3. Ocular instillation into the conjunctival sac of right eye using untreated left eye as control. Single instillation of neat material. Post dose observation period 1, 4, 24, 48 and 72 hours postinstillation and once/day on days 4 and 7. Vehicle: none. Ocular irritation was most prominent at the 1-hour observation when the total Draize scores ranged from 0 to 6 (Maximum possible score = 110). Irritation was confined to the conjunctivae and generally consisted of redness, chemosis and discharge. Corneal ulceration was noted and confirmed using fluorescein stain in one animal at the 24-hour observation. The signs of eye irritation completely subsided in all animals by the day 7 evaluation.
Result	:	Minimal Irritation
Conclusion	:	C11-C14 branched alkyl acetate ester was a mild reversible irritant.
Reliability	:	(1) valid without restriction No circumstances occurred that would have affected the quality or integrity of the data.
Flag	:	Critical study for SIDS endpoint

19.04.2005 (1)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	90 days
Frequency of treatm.	:	once/day
Post exposure period	:	
Doses	:	0, 0.1, 0.5, and 1.0 g/kg/day
Control group	:	yes
NOAEL	:	= 1000 mg/kg
Method	:	EPA OTS 798.2650
Year	:	1985
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)
Remark	:	13-Week Repeated Dose Oral Toxicity on 20 male & female rats. Volume: < or = 1.111 ml/kg (controls received a dose of water volumetrically comparable to the dosage administered to the high dose group, 1.111 ml/kg). Vehicle: none. Clinical laboratory studies (hematology and serum chemistry) were performed pretest on 5 males and 5 females (non-study animals), on 5 animals/sex/dose after 45 days (interim sacrifice), and all animals at study termination. Blood samples were collected from the abdominal aortas following an overnight fast. At 45 days, a complete necropsy was

performed and livers were collected, weighed and preserved. After 13 weeks, all surviving animals were weighed, anesthetized and sacrificed by exsanguination. Complete necropsies were performed.

Result : Liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and do not indicate toxic effects. Microscopic evaluation of the kidneys revealed evidence of mild tubular nephropathy only in the high-dose male rats that were consistent with alpha-2u-globulin effects.

Conclusion : Oral administration of C11-C14 branched alkyl acetate ester daily, 5 days/week for 13 weeks, to rats produced minimal signs of systemic toxicity. There was no treatment-related mortality. The in-life clinical observations were primarily oral and dermal irritation (no clear dose-response). Weekly mean body weights and food consumption values were not significantly altered compared to controls. The qualitative hematologic data were unremarkable at all dose levels. At the terminal sacrifice, glucose values for the 0.5, and 1.0 g/kg/day males were lower than controls and the total protein values for the 1.0 g/kg/day females were higher than controls. Terminal liver and kidney weights were elevated in a dose-related manner but were considered to be adaptive changes and not indicative of toxic effects. Microscopic evaluation of the kidneys showed evidence of mild tubular nephropathy in the mid- and high-dose male rats that were consistent with alpha-2u-globulin effects. Histopathology review of all other tissues from high-dose animals, including reproductive organs (testes, epididymides, prostate, seminal vesicles, ovaries, uterine horns, cervix/corpus of the uterus, and vagina), showed normal morphology. The lowest observable effect level was 500 mg/kg. No effects were observed at 100 mg/kg.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint
19.04.2005 (6)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : other: Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay (Ames Cytogenetic Assay)

System of testing : Bacterial

Test concentration : 156, 312.5, 625, 1250, 2500, 5000, and 10000 µg/plate (312.5 repeat assay only; 5000 and 10,000 initial assay only)

Cycotoxic concentr. :

Metabolic activation : with

Result : negative

Method : other: FIFRA 84-2

Year : 1994

GLP : yes

Test substance : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Remark : Species/Strain: S. typhimurium / TA98, TA100, TA1535, tA1537, TA1538. Species/cell type: Homogenate from the livers of Aroclor 1254 pretreated Sprague-Dawley rats (S9). Vehicle: DMSO.

Result : C11-C14 branched alkyl acetate ester, did not induce significant increases in revertant colonies (> 3 times the vehicle controls) in any of the tested strains with or without metabolic activation in either the initial or repeat assays. The positive control substances produced at least a 3-fold increase in revertant colonies in their respective strains.

In the initial and repeat assay, neither a positive response nor a dose related increase was observed for any of the tester strains. Toxicity, either

a reduction in the number of revertant colonies or a reduction in the background lawn, was not observed. Test substance beading was observed for all tester strains, both with and without metabolic activation at 1250 through 10000 µg/plate. The nontreated and vehicle controls responded in a manner consistent with data from previous assays.

Test condition : There were 2 treatment sets for the assay. One set received exogenous metabolic activation (+S9) and the other saline (-S9). Five tester strains of Salmonella were used: TA98, TA100, TA1535, TA1537, and TA1538. Each of the five strains was dosed with 156, 312.5, 625, 1250, 2500, 5000, and 10000 µg/plate of test substance; a vehicle control (DMSO); a nontreated control and a positive control. Positive controls were tested as follows: 2-aminoacridine (2-AA) at 2.5 µg/plate for all strains with S9; 2-nitrofluorine (2-NF) at 5 µg/plate for TA98, TA1538 without S9; n-methyl-n-nitro-n-nitroguanidine (MNNG) at 10 µg/plate for TA100, TA1535 without S9; and, 9-aminoacridine (9-AA) at 100 µg/plate for TA1537 without S9. There were 3 plates/dose group/strain/treatment set. Samples of bacteria (0.1 ml) followed by 100 µl vehicle, test substance, or positive control substance and 0.5 ml of S9 mix (+S9) or saline (-S9), were added to top agar, vortexed and poured on plates containing a layer of minimal agar medium. Plates were inverted after agar solidification and incubated at 37 ± 2 ºC for approximately 2 days. Plates were evaluated for gross toxic effects and total revertant colony numbers. The initial results of the assay were verified by repeating the assay.

Conclusion : C11-C14 branched alkyl acetate ester was not mutagenic in any strain of Salmonella typhimurium tested and was not toxic in any strain tested under the conditions of this study.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint
19.04.2005 (15)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : other: In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method
Species : mouse
Sex : male/female
Strain : other: Crl:CD-1 (VAF/Plus)
Route of admin. : gavage
Exposure period : 24, 48 and 72 hours
Doses : 0.45, 0.90, and 1.80 grams/kg / Single dose
Result : negative
Method : EPA OTS 798.5395
Year : 1994
GLP : yes
Test substance : other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Remark : The vehicle used was corn oil. Cyclophosphamide (40 mg/kg) in reagent grade water by oral gavage was used as a positive control. Number of animals per sex per dose = 5.

The test substance and the vehicle were administered as a single dose by oral gavage. The vehicle was dosed at a volume equal to the test substance volume. The positive control was administered as a single dose at a volume equal to the test substance volume. Animals from the appropriate groups were sacrificed at approximately 24, 48, and 72 hours. Animals dosed with Cyclophosphamide were sacrificed at 24 hours only. Immediately following sacrifice, both femurs from each animal were

removed and the bone marrow was aspirated, flushed in fetal bovine serum and centrifuged. The cell pellet was resuspended and two slide smears/animal were made. The slides were stained with Acridine Orange and wet mounted. Slides were then evaluated for presence of micronuclei (1000 polychromatic erythrocytes/animal were evaluated).

The test material is considered to be toxic to bone marrow in CD-1 mice based on the decrease in the mean percent of polychromatic erythrocytes at the 48-hour sampling time.

Result : A dose-related decrease in the percentage of polychromatic erythrocytes was observed for the female 48-hour sampling time (regression coefficient $p<0.01$). However, none of the dose groups were statistically different from the control. The positive control (40 mg/kg cyclophosphamide) induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes ($p<0.01$) which indicates that the positive control is clastogenic and is responding in an appropriate manner. Vehicle carrier control values for the mean percent of polychromatic erythrocytes and for the mean percent of micronucleated polychromatic erythrocytes responded in an appropriate manner.

Conclusion : C11-C14 branched alkyl acetate ester did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes in the bone marrow of CD-1 mice. Therefore, it is not considered mutagenic under the conditions of this assay.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint
19.04.2005 (14)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gravid Day 6-15
Frequency of treatm.	:	single dose daily
Duration of test	:	Gravid Day 20
Doses	:	0, 500, 1300, and 2500 mg/kg
Control group	:	other: Sham-Treated with distilled water at 2.5 g/kg
NOAEL maternal tox.	:	= 500 mg/kg bw
NOAEL teratogen.	:	= 2500 mg/kg bw
other: NOEL Maternal	:	= 500 mg/kg bw
other: NOEL Pup	:	= 2500 - mg/kg bw
Method	:	EPA OTS 798.4900
Year	:	1985
GLP	:	yes
Test substance	:	other TS: CAS No. 108419-35-8; Acetic acid, C11-14 methyl-branched alkyl esters, predominantly C13 (40 to 96% C12, C13)

Remark : Developmental Toxicity with 22 mated females per dose. Vehicle: none.

Statistical Methods: Maternal body weight, body weight change, food

consumption, uterine data (i.e., corpora lutea, implants, resorptions), and malformation data were analyzed with Bartlett's test of homogeneity of variance to determine if groups had equivalent variances at the 15 level of significance. If not significantly different, groups were compared using a one-way standard analysis of variance (ANOVA). If significant differences among means were detected, Duncan's test was used to determine the treated group that differed from control. Fetal weights and crown-rump lengths were analyzed using individual fetal values by a standard nested analysis of variance with values nested within dams and dams nested within groups. If differences within groups were indicated, the least-significant-difference technique was used to determine the group(s) that differed from control. If the groups did not have equivalent variances at the 1% level, then a Kruskal-Wallis test (nonparametric) was used to assess differences in group means. If the means were different, a rank sum comparison was used to determine the treatment group that differed from control.

Result : There were no statistically significant deleterious effects on survival, fetal body weight, crown-rump length or malformations at any dose.

Conclusion : C11-C14 branched alkyl acetate ester was administered at 0, 500, 1300, and 2500 mg/kg on gestation days 6-15 in a developmental toxicity study in rats. Maternal toxicity was seen at the 1300 and 2500 mg/kg doses as evidenced by decreases in body weight. There were no statistically significant deleterious effects on fetal survival, body weight, or crown-rump length and no evidence of treatment-related malformations.

Reliability : (1) valid without restriction
No circumstances occurred that would have affected the quality or integrity of the data.

Flag : Critical study for SIDS endpoint
19.04.2005 (4)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bio/dynamics Inc, East Millstone, NJ; Project # 330613.

(2) Bio/dynamics Inc., East Millstone, NJ, Acute Dermal Toxicity Study in the Rabbit; Project # 330606.

(3) Bio/dynamics Inc., East Millstone, NJ, Oral Gavage Probe Study in the Rat; Project # 252171.

(4) Bio/dynamics Inc., East Millstone, NJ, Oral Teratology Study in Rats; Project # 352134.

(5) Bio/dynamics Inc., East Millstone, NJ, Primary Dermal Irritation Study in the Rabbit; Project # 330604.

(6) Bio/dynamics Inc., East Millstone, NJ, Subchronic Oral Gavage Study in Rats; Project # 252170.

(7) Bio/dynamics, East Millstone, NJ, Acute Oral Toxicity Study in the Rat; Project # 330601.

(8) BioDynamics Inc. 1985. A Flow-Through Acute Fish Toxicity Test. Study #252141.

(9) BioDynamics, Inc. 1985. An Acute Algal Toxicity Test. Study #252159.

(10) BioDynamics, Inc. 1985. Ultimate Biodegradability. Study # 252189.

(11) EPIWIN (1999). Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(12) EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

(13) Exxon Biomedical Sciences, Inc. 1985. An Acute Static Daphnia Toxicity Test. Study # 252142A.

(14) Exxon Biomedical Sciences, Inc., East Millstone, NJ, In Vivo Mammalian Bone Marrow Micronucleus Assay Oral Gavage Dosing Method, Project # 168930.

(15) Exxon Biomedical Sciences, Inc., East Millstone, NJ, Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay; Study # 168925.

(16) ExxonMobil Chemical Company (2003). Exxate 1300 Data Sheet.

(17) Mackay D (1998). Level I Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT